# HYDROXYLASES AND MODULATORS THEREOF

## Field of Invention

The present invention relates to methods of designing inhibitors of FIH using the crystal structure of FIH, and to inhibitors of FIH and their use in the treatment of ischaemia.

## Background of the Invention

In cells of many organisms exposure to an environment in which oxygen is depleted relative to optimal levels induces a hypoxic response. In these hypoxic cells, activation of a transcriptional cascade involving hypoxia inducible factor (HIF) directs a series of adaptive responses that enhance oxygen delivery or limit oxygen demand. Activation of HIF in cancer and ischaemic hypoxic vascular diseases has revealed its important role in human pathology and demonstrated that manipulation of HIF activity has important therapeutic potential.

The HIF transcriptional complex comprises an αβ heterodimer, HIF-β being a constitutive nuclear protein that dimerises with oxygen regulated HIF-α subunits (Semenza, G. L. (2000) *Genes Dev.* **14**, 19831991). The activity of HIF-α, is suppressed by oxygen-dependent modification catalysed by a series of $Fe^{(II)}$ and 2OG dependent dioxygenases that hydroxylate specific HIF-α residues. In the presence of oxygen in human HIF-1α, 4-hydroxylation of Pro402 or Pro564 by a set of HIF prolyl hydroxylase isozymes (PHD1-3) (Epstein et al. (2001) *Cell* **107**, 4354; Bruick, R. K., and McKnight, S. L. (2001) *Science* **294**, 13371340) mediates its recognition by the von Hippel-Lindau (VHL) ubiquitin ligase complex and consequent targeting for proteasomal destruction (Ivan et al, (2001) *Science* **292**, 464468; Jaakkola et al (2001) *Science* **292**, 468472, WO 02/074981). In a complementary mechanism FIH catalyses β-hydroxylation of HIF-1α Asn803 (Lando et al, (2002) *Science* **295**, 858861) blocking interaction with the transcriptional co-activator p300 (Dames et al., (2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 52715276; Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 53675372). In hypoxia, limitation of enzymatic activity allows HIF-α to escape destruction and become transcriptionally active.

Inhibition of HIF hydroxylases strongly activates the HIF transcriptional cascade even in the presence of oxygen (Epstein et al.(2001) *Cell* **107**, 4354). Thus, inhibition of the HIF hydroxylases results in a pro-angiogenetic response that may be used in the treatment of cardiovascular diseases/ ischaemic hypoxic vascular diseases including myocardial infarction and anaemia. A problem with this approach is that the human cells contain other enzymes belonging to the same family as the HIF hydroxylases, i.e. utilising dioxygen (a cosubstrate), 2-oxoglutarate (2OG) (a cosubstrate) and Fe(II) (a cofactor). Such enzymes are exemplified by phytanoyl coenzyme A hydroxylase, procollagen prolyl-4-hydroxylase, procollagen prolyl-3-hydroxylase, gamma-butyrobetaine hydroxylase, Alk B (a DNA repair enzyme) and others including predicted 2OG oxygenases identified on the basis of sequence analyses including a sub-family related to FIH (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). It is generally agreed that it is desirable that enzyme inhibitors used as pharmaceuticals are selective for their intended target or the targets involved in producing the desired effect. A lack of selectivity can lead to toxic side effects that render particular compounds unsuitable for use in human or animal therapy. One approach to identifying compounds that are selective for the intended target is to undertake structural, mechanistic and other analyses on the intended agents and to use the information gained to aid in the preparation of selective compounds, or more selective compounds (relative to those previously known), for use as pharmaceuticals for use in humans or animals. Here we describe structural and other studies on the HIF hydroxylases that enable the design of selective inhibitors of FIH and related enzymes.

## Summary of the Invention

The present inventors have now identified the site of hydroxylation of asparagine 803 of HIF-1α by FIH. In addition, the inventors have obtained the crystal structure for FIH including identification of the binding site and residues involved in the interaction of FIH with HIF.

Accordingly, the present invention provides a method of identifying, screening, characterising or designing a chemical entity which mimics or binds to FIH, which method comprises comparing a structural model of FIH with a structural

model for said chemical entity, wherein said structural model of FIH is derived from structural factors or structural coordinates determined by subjecting to X-ray diffraction measurements a crystal comprising FIH.

The invention also provides for:

- the use of the structural co-ordinates obtainable by subjecting a crystal comprising FIH to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity;
- a chemical entity identified by a method of the invention, wherein said chemical entity inhibits the asparaginyl hydroxylase activity of FIH; and
- a chemical entity of the invention for use in a method of treatment.

Description of the Figures

Figure 1: 2OG binding site.

Figure 2: binding of Asn-803.

Figure 3: conformation of CAD at site 1.

Figure 4: conformation of CAD at site 2.

Figure 5: figure indicating the turn formed by 802-804 of HIF-CAD at the active site of FIH.

Figure 6: conformation of the turn formed by residues 802-804 of HIF-CAD at the active site of FIH.

Detailed Description of the Invention

The present inventors have identified the position of asparagine 803 that is hydroxylated by FIH. In addition, the inventors have identified the crystal structure of FIH. This structure therefore allows for identification of the amino acid residues involved in binding of FIH to HIF.

The identification of the interaction and the structures allows for the characterisation or identification of chemical entities which can bind and in particular which can inhibit FIH. A number of different types of inhibitors can be identified as discussed in more detail below.

The inventors have successfully crystallised human FIH. This the first crystallisation of FIH and has enabled determination of the crystal structure. Co-ordinates from the crystal analysis are set out in Table 3 below. The studies have allowed analysis of the binding of asparagine-803 of HIF and analysis of the conformation of the c-terminal activation domain (CAD) of HIF at the binding sites to FIH. The present invention provides the use of the structural co-ordinates of FIH to identify, characterise, design or screen chemical entities. The chemical entities of interest are those which bind to FIH and in particular which inhibit the asparaginyl hydroxylase activity of FIH. In addition, chemical entities may be identified, characterised or designed which are modified asparagine hydroxylases.

Typically, the structural co-ordinates used are obtainable by subjecting a crystal comprising FIH or a fragment thereof to X-ray diffraction measurements and deducing the structural co-ordinates from the diffraction measurements, to identify, screen, characterise, design or modify a chemical entity. The structural co-ordinates indicate the positions of individual atoms within the crystal and give an indication of the space available for adjusting the position of individual atoms when designing a chemical entity.

The crystal subjected to X-ray diffraction methods comprises FIH or a fragment thereof. The FIH may be from any source but is preferably human FIH. The FIH may be a modified form. For example, the FIH may be modified by insertion, deletion, n-terminal or C-terminal addition, or substitution of amino acid by another amino acid. Amino acid substitutions may be conservative substitutions. Typically, when crystallised, a FIH mutant will adopt a similar 3-dimensional structure to that adopted by the corresponding FIH. A mutant may be an inactive FIH.

References to FIH herein refer to FIH and homologues thereof. Amino acid residues are defined with reference to the position in FIH (see e.g. Hewitson et al). The relevant amino acid residues of homologues of FIH are the equivalent amino acid residues, based on for example the best alignment of homologue to FIH.

A FIH may be isolated by any suitable means for use in crystallisation studies. For example, a FIH may be purified using biochemical means from a suitable source. Typically, however, it will convenient to over express FIH in cells and purify FIH from those cells. Thus, a polynucleotide encoding a FIH may be used

in the construction of a vector. The FIH may be crystallised according to any method known to those skilled in the art. X-ray diffraction may be carried according to any suitable method. The data collected from X-ray diffraction experiments may be processed to deduce the structural co-ordinates of FIH using any suitable method.

The invention provides the use of structural co-ordinates to identify, characterise, design or screen a chemical entity. The chemical entity may be one which binds to FIH, or which acts as an inhibitor of asparaginyl hydroxylase activity. Alternatively, the chemical entity may be a modified FIH to alter the activity of a FIH.

A chemical entity which binds to or inhibits FIH is any chemical entity capable of forming an association with the FIH. The binding or inhibition may be non-specific, for example, such an entity may also bind to or inhibit other 2OG oxygenases. Alternatively, an agent may be designed or identified which specifically binds to or inhibits asparaginyl hydroxylases. An agent may be designed or identified which is a specific inhibitor of FIH, but not other asparaginyl hydroxylases.

The structural co-ordinates of FIH allows a skilled person to predict which amino acids are important in active site formation and which amino acids are important in contacting the substrate. The substrate binding site may be shown as a 2 dimensional representation or a 3 dimensional representation produced by physical models or displayed on a computer screen. Such representations can be used to design, identify or screen chemical entities which bind to or inhibit or are predicted to bind to or inhibit FIH. Such representations can also be used to identify modifications of FIH to alter its activity characteristics.

Examples of modifications to FIH include modifications to increase the binding of FIH for its substrate, or to alter the substrate the specificity. Alternative modifications include those which alter the activity of FIH, for example, to remove asparaginyl hydroxylase activity.

The representations of the structures may be used in other ways. For example, the representations of the FIH active site may be used to model constraints by the putative introduction of covalent bonds between the atoms which come close together when FIH binds to a substrate. Representation of the active site may be used to predict which residues of FIH are likely to be involved in steric hindrance.

Such residues may be modified, replaced or deleted to decrease esoteric hindrance in order to increase avidity of the peptide for its substrates.

In general, it will be necessary to process the structural co-ordinates obtainable according to the invention in computer-based methods in order to identify or design chemical entities with the desired molecular structure or to identify chemical entities whose structure is complementary to all or part of another chemical entity of interest. Thus, chemical entities which have a structure similar to FIH may be identified or designed. Chemical entities which bind to FIH may be identified or designed. Preferably, such chemical entities bind at the active site of FIH and in general may act as inhibitors of asparaginyl hydroxylase activity.

Such computer-based methods fall into two broad classes: database methods and *de novo* designed methods. In database methods, the chemical entity of interest is compared to all chemical entities present in a database of chemical structures and chemical identities whose structure is in some way similar to the compound of interest identified. The structures in the database are based either on experimental data, generated by NMR or X-ray crystallography, or models of 3 dimensional structures based on 2 dimensional data. In *de novo* design methods, models of chemical entities, for example such are those which might bind to FIH are generated by a computer program using information derived from known structures and/or theoretical rules.

Similarly, the FIH structural coordinates may be used to screen for the expected activity of chemical entities selected, designed or shown to be modulators such as inhibitors of other hydroxylases, for example prolyl hydroxylases. For example the compounds may be screened to assess the likelihood of a prolyl hydroxylase inhibitor additionally inhibiting FIH hydroxylase. Such screening methods may be useful in identifying agents which selectively inhibit HIF prolyl hydroxylase, but not HIF asparaginyl hydroxylase.

Chemical entities designed or selected according to the methods of the invention may be tested and optimised using computational or experimental evaluation. Experimental methods to assay for the activity of asparaginyl hydroxylase are described in more detail below.

Based on the structure of FIH, a number of different types of inhibitors can be identified. These inhibitors are discussed in more detail below.

Dimerisation inhibitors

The crystallographic asymmetric unit contains one FIH molecule. However, analysis of crystallographic symmetry revealed a dimeric form of FIH, consistent with native gel-electrophoresis analysis. The dimer interface involves the two C-terminal helices of each molecule in an interlocking arrangement predominantly involving hydrophobic interactions. This unusual interface buries a surface area of 3210 $Å^2$, large on average by comparison to other dimeric proteins of this size. Inhibitors of dimerisation include those that bind to residues that form the dimerisation interface including residues selected from 330-346, such as Leu-340 and Ile-344. Inhibitors include peptides or peptide mimetics that correspond to all or part of the FIH residues involved in the dimerisation interface.

For example, such inhibitors may comprise a fragment of FIH, for example, including the residues from 340 to 344, preferably, including residues 330 to 346. Such a fragment may typically have 6 or 10 amino acids in length, preferably, up to 15 or 20 amino acids in length. Alternatively, peptide homologues may be used, for example, which comprise a homologue to the residues of 340 to 344 or 330 to 336, including 1, 2 or more substitutions. Additional agents include peptides or peptide mimetics which can be designed based on the crystal structure to interfere with dimerisation.

Inhibitors exploiting metal binding in FIH:

The structural work defines the presence of Fe(II) at the active site of FIH and by implication related HIF hydroxylases. The iron is bound in an almost octahedral manner by the side chains of His199, Asp201 and His279, the 2-oxo and 1-carboxylate groups of 2OG. In the enzyme-substrate complexes there is a vacant position opposite His279 revealing that the enzyme is primed for dioxygen binding. Accommodation of a ligand opposite His279 may require disruption of the hydrogen bond between Asp201 and CAD Asn803 (the iron and Asn803 β-carbon are only ~4.9 Å apart). Subsequent decarboxylation of 2OG presumably yields an iron-oxo

species [$Fe^{(IV)}$=O <–> $Fe^{(III)}$-O·] that effects oxidation at the carbon of Asn-803 in the C-terminal transactivation domain (CAD) of HIF.

Compounds that contain functional groups that bind to iron are useful as inhibitors of FIH. Examples of such compounds include thiols, alcohols, phenols including flavonoids such as quercitin and derivatives thereof, carbohydrates, hydroxamates, imidazoles and other heterocycles for example nitrogen containing heterocycles.

$Zn^{(II)}$ binds to FIH in an identical manner to $Fe^{(II)}$ (structure 3), consistent with the metal-mediated hypoxic effect being due to displacement of $Fe^{(II)}$ from the active site of HIF hydroxylases. Since neither Zn(II) nor other metal inhibitors of FIH can replace Fe(II) as a cofactor in catalysis, compounds that preferentially promote the binding of a metal other than iron [such as Zn(II)] at the active site of FIH act as inhibitors.

A further class of inhibitor are non-metallic inhibitors that operate via competing with Fe(II) for binding at the active site. Such inhibitors may bind to any or all of the triad of residues (His-199, Asp-201, His-279), that bind the Fe(II) at the active site of catalytically active FIH.

Inhibitors exploiting the 2OG binding sites

The FIH:CAD structures with NOG reveal that like 2OG it is ligated to iron in a bidentate manner and imply it is an inhibitor due to decreased susceptibility to attack by an iron bound (su)peroxide intermediate or by hindering binding of dioxygen to the metal.

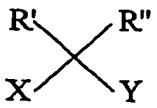
The structural studies on FIH reveal the binding interactions for the 2OG and NOG (see for example Figure 1). The 5-carboxylate of 2OG (and the equivalent carboxylate of NOG) forms hydrogen bonds with the side-chains of Lys214, Thr196 and Tyr145; such interactions are unprecedented in other structures of 2OG oxygenases. FIH is further unusual in that Lys214 is on the fourth DSBH (double stranded beta-helix) β-strand whereas previously assigned basic 2OG-5-carboxylate binding residues are at the beginning of the eighth DSBH strand.

The structural studies reveal the FIH residues that form the pocket into which 2OG and NOG bind. In addition to the aforementioned these include the side-chains

of Ile-281, Leu-186, Leu-188, Phe-207, Thr-196. Knowledge of these interactions enables the design of improved (as measured by binding parameters) and selective inhibitors. Thus, for example an inhibitor binding in the 2OG binding pocket may form hydrophobic interactions with any or all of the side chains of Ile-281, Leu-186 Leu-188, Phe-207, Thr-196. Further it may form electrostatic or hydrogen bonding interactions with the residues involved in binding the 5-carboxylate of 2OG (Lys214, Thr196 and Tyr145).

Selective inhibition of FIH via inhibitors interacting with the 2OG binding residues is exemplified as follows: kinetic analyses of a series of inhibitors based upon *N*-oxaloyl amino acids revealed the *R*-enantiomer ($IC_{50}$ 0.4 mM) of *N*-oxaloylalanine was significantly more potent than the *S*-enantiomer ($IC_{50}$ 2.5 mM). Analysis of the 2OG binding pocket in FIH reveals that the binding of the S-enantiomer is hindered by interactions between its methyl group and the side chain of Thr-196 and, Ile-281 in the 2OG binding pocket. A reversed selectivity (i.e. the S-enantiomer was more potent) was observed both for procollagen prolyl-hydroxylase and the PHD isozymes, demonstrating it should be possible to develop selective inhibitors for individual types of HIF hydroxylase. Such inhibitors may or may not chelate to an active site metal.

Compounds include those of general formula

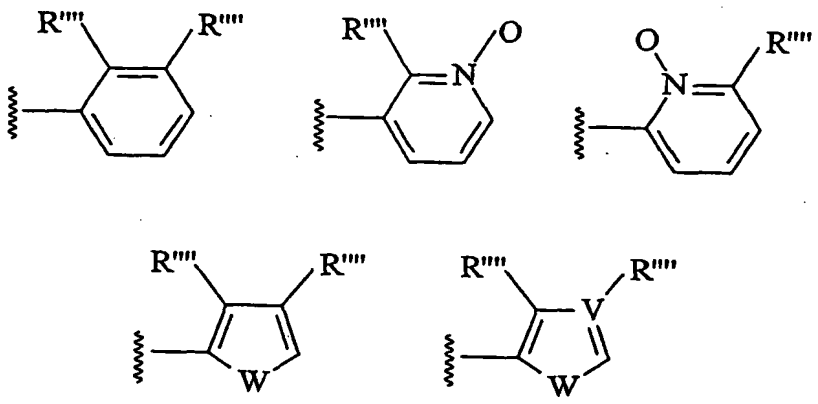



(I)

wherein each of R′ and R", which may be the same or different, is H, F or $C_1$ to $C_3$ alkyl or substituted alkyl, $CH_2OH$, $CH_2CO_2H$ or $CONH_2$, X is COOH, SOOH, or CONHH or an ester thereof, or heterocyclic or other group which forms a favourable interaction with one or more of the side chains of Lys-214, Thr-l96 and Tyr-l45, i.e. those residues involved in binding the 5-carboxylate of 2OG as revealed in the crystallographic analyses,

Y is - $(CR'''R''')_nZ$, where Z is

- NR'''COCOOH, -NR'''CSCOOH, - NR'''COCOSH,
- CHSR'''CONR'''R'''', -CHOR'''CONR'''OR''', - CHSR'''CONR'''OR''' or
- CHOR'''CONR'''NR'''OR''', wherein each R''', which may be the same or different, is H, alkyl, OH or O-alkyl, n is 0 to 3 and preferably 0, or



wherein R'''' is OH, OR''' or NHCOR''', and W is S, NH, or O.

Thus X is a group that forms favourable interactions with one or more of the side chains of interactions one or more of the side chains of Lys-214, Thr-196 and Tyr-145, i.e. those residues involved in binding the 5-carboxylate of 2OG. X may be functionalised as a pro-drug such that is delivered to the desired site of action or has desirable pharmokinetic properties. As indicated above, X can be an ester such a methyl or ethyl ester or amide derivative of carboxylic acid versions of X.

If n is 0, Y is typically CONHOH, $CONHNH_2$, NR'''COCOOH, NR'''CSCOOH or NR'''COCOSH. Y is preferentially of a size such that it can chelate to the active site metal whilst maintaining all or some of the favourable binding interactions found in the 2OG binding pocket as defined by crystallographic analyses. As with X, Y may be functionalised as a pro-drug.

When Y contains an aromatic ring as indicated above it can comprise other ring systems including aryl or functionalised aryl rings as well as heterocyclic and functionalised heterocyclic rings. The above rings may be further functionalised to optimise binding at the FIH active site.

Inhibitors exploiting the peptide substrate binding site

There are two binding sites

The ES complex structures unexpectedly reveal two separate binding sites involving $CAD_{795-806}$ (i.e residues 795-806 of the C-terminal transactivation domain of HIF) (Site 1) and $CAD_{813-822}$ of HIF (Site 2) with contact surface areas of 1640 $Å^2$ and 1080 $Å^2$, respectively (see for example the figures). CAD residues in these regions are conserved in all known HIF-1α and HIF-2α sequences. The electron density for site 1 was of good quality, with only the side-chain of Tyr798 poorly defined, while that for site 2 was at a lower level and quality, probably reflecting weaker binding at this site. $CAD_{804-806}$ and presumably also $CAD_{807-811}$, for which density was not observed, do not form direct interactions with FIH. Kinetic analyses employed to investigate the relative importance of Sites 1 and 2, revealed that fragments containing site 1 only are hydroxylated by FIH but less efficiently than those containing both sites demonstrating that both are important in binding and that both may be exploited in inhibition studies.

At Site 1 $CAD_{795-803}$ are bound in a groove and adopt a largely extended conformation linked to FIH by ten hydrogen bonds. Asn803 of CAD is strikingly buried at the active and directly adjacent to the $Fe^{(II)}$. CAD Asn803 and Ala804 form a tight turn, stabilised by a hydrogen bond between the backbone carbonyl of Val802 and NH of Ala804, which projects the side chain of Asn803 towards the $Fe^{(II)}$. The side chain of CAD Asn803 is precisely orientated by three hydrogen bonds to enable hydroxylation at the *pro-S* position of the β-carbon consistent with the NMR assignments (see above) The primary amide of CAD Asn803 is sandwiched between FIH residue Tyr102 and the $Fe^{(II)}$, and forms hydrogen bonds with the side chains of FIH residues Gln239 and Arg238 , residues located on the insert to the DSBH motif. Significantly, the substrate and $Fe^{(II)}$ binding sites are directly linked since the backbone nitrogen of CAD Asn803 also forms a hydrogen bond (~3 Å) with the carboxylate oxygen of Asp201 that is not complexed to the iron. Six additional hydrogen bonds stabilise the binding of FIH to $CAD_{795-801}$.

In contrast with Site 1, Site 2 is located on the FIH surface and involves only two hydrogen bonds. $CAD_{816-823}$ of Site 2 form an α-helix, in exact agreement with the structure of this region in complex with CBP/p300 (Dames et al., (2002) *Proc.*

*Natl. Acad. Sci. U. S. A.* **99**, 52715276; Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 53675372). As in that complex, the highly conserved Leu818, Leu819 and Leu822 sit in a hydrophobic pocket on the surface of FIH and form the basis of the binding interaction and so it is not possible for these residues to bind simultaneously to CBP/p300 and FIH.

The extended loop conformation adopted by the CAD residues at Site 1, contrasts with the α-helical conformation adopted by the same residues when complexed with the 1st transcriptional adaptor zinc-binding domain (TAZ1) of CBP/p300(Dames et al.,(2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 52715276; Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 53675372). The disordered structure observed for the CAD, and other HIF-α residues, when free in solution may thus reflect a requirement to adopt more than one conformation for complex formation with different proteins.

The changes in the conformation of CAD on binding are complemented by changes in FIH revealing an induced fit binding process; Trp296 of FIH undergoes a 50° rotation about $C_{beta}$-$C_{alpha}$ to accommodate CAD Val802, while both Tyr102 and Tyr103 become more ordered. Further evidence of induced fit comes from the significant differences in resolution between the structures obtained with and without CAD fragments bound reflecting ordering of FIH that occurs on binding (structure 4, for comparison, represents FIH complexed with $Fe^{(II)}$ and 2OG alone). Interference in the conformational changes involved in the hypoxic response, in particular those involving the CAD region, e.g. by use of small molecules or by gene or protein therapy, may allow manipulation of the hypoxic response to enable pro or anti-angiogenetic responses.

Thus, the structural studies define the (i) FIH residues involved in binding the CAD of HIF (ii) conformation of FIH when CAD is bound and (iii) conformation of CAD when bound to FIH. These results are useful in the design of selective inhibitors of FIH and related enzymes. Features of the FIH binding sites may be used to mediate tighter binding of inhibitors to FIH or to obtain inhibitors that do not bind tightly to FIH, i.e. avoid inhibition of FIH.

Inhibitors binding at or close to the Site 1 may exploit electrostatic, hydrogen binding and/or hydrophobic interactions with Tyr-102, Asp-104, Lys-106, Asp-201,

Glu-202, Gln-147, Gln-239, residues 299-303, His-313, Ala-317, Ile-318, Asn-321, Lys-324, Arg-238, Trp-296, Asn-321- Lys-324. Inhibitors binding at Site 1 may mimic or partially mimic the turn conformation adopted by CAD when bound at Site 1.

Inhibitors binding at or close to Site 2 may exploit electrostatic, hydrogen binding and/or hydrophobic interactions with residues Thr-149, Leu-150, Asn- 151, Asp-152 and residues Val-159, Phe-162, Leu-163, Trp-167, Gln-181, Leu-182, Thr-183, Ser- 184, Asn- 185. Inhibitors binding at Site 2 may mimic or partially mimic the helical conformation adopted by CAD when bound at Site 2.

It is recognised that inhibitors need not bind to both Sites 1 and 2, although that they may, and that Site 1 is preferred over Site 2.

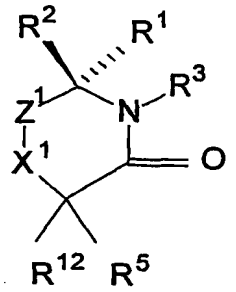
Residues 801 – 805 of CAD that bind at Site 1, and in particular residues 802-805 form a turn conformation in which the distance of the backbone C=O of 802 to the backbone NH of 804 is ca. 2.8 Å. Including the H-bond formed between the NH of Ala-804 and the carbonyl O of Val-802 of the HIF-1alpha CAD, the turn contains 7 atoms in a pseudo-ring.

Turns are especially amenable to mimicry by analogues useful for enzyme inhibition or receptor binding. The medicinal chemistry literature is replete with examples of such turn mimics. These can be modified by known methods to bind to specific targets, in particular given the knowledge of the target structure.

Examples of turn mimics and their modifications can be found in the following reviews: Hanessian et al, TETRAHEDRON 53: 12789-12854 SEP 22 1997; Gillespie et al, BIOPOLYMERS 43: 191-217 1997; and Burgess et al., ACCOUNTS CHEM RES 34: 826-835 2001). Recent examples of primary reports on turns include the following (and references therein) Maier et al, EUR J ORG CHEM: 2686-2689, 2002; Reid et al, J AM CHEM SOC 124: 5673-5683, 2002; Mahadevan et al, J BIOMOL STRUCT DYN 19: 775-788 2002; Eguchi et al, J MED CHEM 45: 1395-1398 2002; De Borggraeve et al, TETRAHEDRON LETTERS 42: 5693-5695 2001; Kohn et al, TETRAHEDRON LETT 42: 4453-4457 2001; Eguchi et al, TETRAHEDRON LETT 42: 1237-1239 2001; Manzoni et al, TETRAHEDRON 57: 249-255 2001; Jiang et al., HELV CHIM ACTA 83: 3097-3112 2000; Derrer et al, J CHEM SOC PERK T 1: 2957-2967 2000; Belvisi et al,

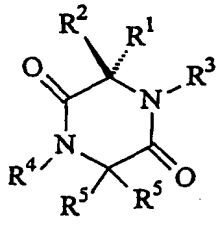
EUR J ORG CHEM: 2563-2569 2000; Claridge et al, BIOORG MED CHEM LETT 6: 485-490 1996.

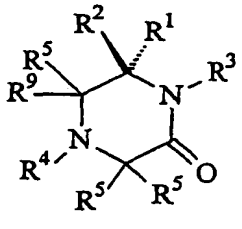
These include compounds of the general formula:

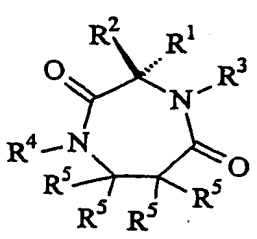


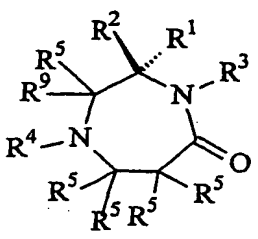
II

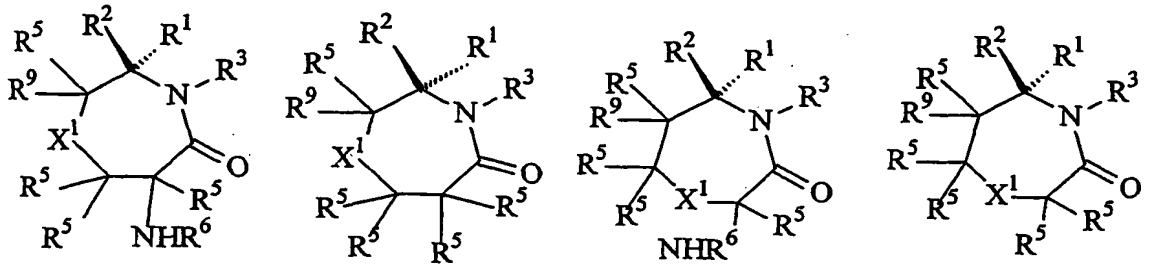
wherein $R^1$ is such that it can form an electrostatic or H-bonding interaction with Gln-237 and or Arg-238, preferably $CR^8R^9CONH_2$ or an analogue thereof where $R^8$ is hydrogen or a peptide or peptide mimetic (such as those composed of β-amino acids or peptide isoteres), and $R^9$ is hydrogen, optionally functionalised alkyl, optionally functionalised aryl, heteroaryl or any combination thereof such as $CH_2CONH_2$, $R^2$ is hydrogen or a group that will interact favourably with Tyr-102 of FIH, $R^3$ is H or a group which can form a H-bond with Asp-201, $Z^1$ is $\rangle C{=}O$ or $\rangle CR^5R^9$ where $R^5$ is hydrogen, optionally functionalised alkyl, aryl, or heteroaryl or any combination thereof, $R^{12}$ is as defined for $R^5$ or is $NHR^6$ where $R^6$ is $COR^5$ or $SO_2R^5$and $X^1$ is $NR^4$, $NR^4C(R^5)_2$, $C(R^5)_2NR^4$, or O or NH where $R^4$ is $COR^5$ or $SO_2R^5$. In this and in the other formulae each $R^1$, $R^2$, $R^3$, $R^4$, $R^5$, $R^6$, $R^7$, $R^8$, $R^9$, $R^{10}$, $R^{11}$ and $R^{12}$ can be the same or different. In particular, these compounds may have one of the formulae





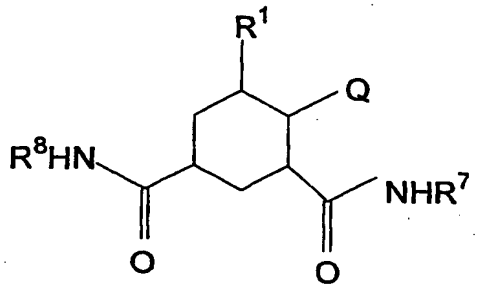






wherein the radicals are as defined above, and $R^7$ and $R^8$ are independently peptides or peptides mimetics or part peptide mimetics, such as those containing or consisting of beta-amino acid residues, urethane, sulphonamide or phosphonamide links.

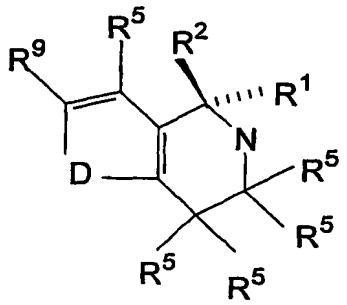
Other compounds which can be used are those possessing the formula



III

where Q represents H or OH and $R^7$ and $R^8$ are as defined above.

Further compounds which can be used possess the formula



IV

wherein $R^1$, $R^2$, $R^5$ and $R^9$ are as defined above and D is S, O, NH or $CHR^9=CHR^9$. Thus the ring attached to the six-membered ring is either a five-membered heterocyclic ring or an aryl ring.

In these formulae $R^8$ and $R^9$ can be optimised to bind in the channel linking the 2OG and peptide substrate binding sites and to the 2OG binding site itself.

Cyclic peptides acting as mimics of the turn adopted by CAD in site 1. The cyclo may be formed via peptide links, disulphide bonds or C-C bonds.

Inhibitors employing a combination of binding sites

It is well known that enzyme inhibitors competing for binding at more than one substrate or cosubstrate binding site, sometimes termed bisubstrate inhibitors, can be useful. Examples can be found in Wang et al, BIOCHEMISTRY-US: 15676-15683 2001; and Lerner et al, ANGEW CHEM INT EDIT 40, 4040-4041, 2001.

In the case of FIH and other 2OG oxygenases bisubtrate inhibitors may be useful since features of 2OG binding may be present in more than one enzyme whereas the CAD substrate is unique. Thus, inhibitors that bind to both binding sites may show improved selectivity over those that bind to the 2OG binding site only. The structural analyses enable the identification of such bisubtrate inhibitors. The 2OG and CAD binding sites are linked to each other via a 'channel' extending from the 2-oxo group of 2OG (or NOG) to the beta-carbon Asn-803 in the FIH.Fe.2OG/NOG.HIF(CAD) complexes. In the structures this 'channel' either appears empty but may be occupied by water molecules. The distance from the C of the 2-oxo group of 2OG to the beta-C of Asn-803 is ca. 6 Å. The distance from the 3-C of 2OG to the beta-C of Asn-803 is ca. 6.6 Å. The information from the structural analyses enables the identification of bisubstrate inhibitors, including the following:

These are compounds of formulae (II) to (IV) as defined above except that they are modified such that they can also bind into the 2OG binding pocket as defined by the crystallographic information. Thus, either $R^2$ or $R^1$ is modified such that they can bind into the 2OG binding pocket. The modification takes the form such that the general formula of $R^1$ or $R^2$ is A-X where X is as defined above and A links X to (II). A is of appropriate length such that X can bind to formula 1 the residues of the 5-

carboxylate of 2OG as discussed above under the heading Inhibitors Exploiting the 2OG binding sites.

More generally bi-substrate inhibitors of FIH can have the formula:

X [B]-[C]

where X is as defined above, B is a linker group and C is an entity binding to part of the CAD binding site of FIH, in general $CONH_2$.

B is typically a polymethylene group, generally having 6 to 8 carbon atoms or an equivalent group where one or more of the carbon atoms is replaced by a heteroatom, notably O, S or N and can be functionalised, for example with thiol, alcohol, carboxylate, hydroxamic acid or oxalate to mediate Fe binding. It is preferably 6 to 8 carbon atoms long or its equivalent. Alternatively, B is a linking group which possesses a ring, preferably of 5 to 7 members to which C is attached.

Inhibitors that bind to the 2OG binding site or part thereof and the peptide substrate

Another class of inhibitors bind to the enzyme-substrate complex, i.e. to FIH.Fe(II).HIF(CAD). The structural analyses enable the identification of such inhibitors. As described above 2OG and CAD binding sites are linked to each other via a 'channel' extending from the 2-oxo group of 2OG (or NOG) to the beta-carbon of Asn-803 in the FIH.Fe.2OG/NOG.HIF(CAD) complexes.

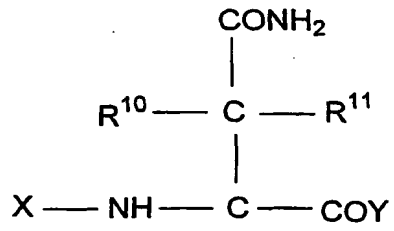
Inhibitors of this type may be defined as X-[B]-[E] where X is as defined above, B is a linker group such as defined above and E is an entity binding to part of the CAD when bound to HIF. E may bind to the backbone carbonyl oxygen of Asn-803 of CAD and to the $NH_2$ group of the primary amide of Asn-803.

Mechanism based inhibitors

Another class of inhibitors is based upon substrate analogues that can undergo part of the catalytic cycle but either stall at an intermediate stage or cause an aberrant reaction resulting in damage or inhibition. The observation that FIH catalyses hydroxylation of Asn-803 at the beta-position together with the structural analyses enables the design of such inhibitors. Such compounds include analogues of the

substrates (inhibitors) in which Asn-803 is replaced with an analogue which does not undergo oxidation such as beta-fluoro- asparagine, beta-di-fluoro- asparagine, beta-methyl- asparagine, beta-dimethyl- asparagine derivatives. Alternatively derivatives that undergo oxidation to give an agent that can be oxidised to give an inactivating group such as an epoxide or metal chelating group may prepared (such mechanism based inhibitors are sometimes referred to as suicide inhibitors). In the case of FIH they include alpha-beta-dehydroasparagine and beta-methylene asparagine.

These include a compound having the formula



wherein X represents a valine residue or an analogue thereof and Y represents an alanine residue or an analogue thereof, $R^{10}$ is fluorine or $C_1$ - $C_3$ alkyl, especially methyl, and $R^{11}$ is fluorine, $C_1$ - $C_3$ alkyl or hydrogen i.e. the specified residue is β-mono- or di-fluoroasparagine or β-mono- or di-methylasparagine.

Alternatively, the compound above may be desaturated, i.e. is an alpha/beta dehydroamino acid ($R^{11}$ not present) or $R^{10}$ and $R^{11}$ may be replaced by a methylene group, i.e. the residue is α, β-dehydro-asparagine or β-methylene asparagine.

If desired the valine residue is connected to one or more units of the peptide DESGLPQLTSYDCE - in the order given e.g. to glutamic acid (E) alone or to, for aspartic acid (D) - cysteine (C) - glutamic acid (E)-, or a longer chain such as PQLTSYDCE -.

For the compounds of this invention suitable aryl rings include phenyl and napthalenyl, which may be further functionalised or fused to other ring systems. Suitable heterocyclic rings include thiophene, pyridine, quinoline, isoquinoline, pyrimidine, pyrazine, pyrone, chromone, coumarin, indole, isoindole, indolizine, benzofuran, pyridazine, purine, oxazole, pyrazole, isothiazole, pyrrolidine,

piperidine, indoline, benzothiaphen, morpholine, benzimidazole, azepine, azacine, azoine, oxepine, oxocine, oxoine, piperazine, oxazine, thiazine, thiepine, thiocine, thioine, furan, imidazole, azole, diazole, triazole and tetrazole ring systems that may be functionalised or fused to other ring systems.

The said alkyl and aryl groups and chains are typically functionalised by alcohol, fluorine, thiol, a carboxylic acid, phosphonic or phosphinic acid, sulphonic acid or other chelating group, in the case of the chains typically via an alkyl group. In the formulae described herein, a branched or straight $C_1$ to $C_6$ alkyl chain may be a methyl, ethyl, propyl, butyl, iso-butyl, *tert*-butyl, pentyl, neopentyl, *tert*-pentyl or a primary, secondary or tertiary hexyl group. Preferably the alkyl groups are methyl, the preferred heterocyclic rings are pyrolidine and tetrahydropyran and the preferred aromatic rings are benzene, naphthalene and pyridine.

The compounds which are acids can be present in the form of salts, such as sodium salts.

The crystal structure of FIH also allows identification of those residues involved in asparaginyl hydroxylase activity of FIH. The crystal structures may therefore be used to design modified FIH, for example, which has reduced or no asparaginyl hydroxylase activity, for example, by mutation of critical residue within the active site. In the alternative, those residues involved in substrate binding can be identified and modified, for example, to allow the asparaginyl hydroxylase to accept other substrates than HIF. For example, by enlarging or decreasing the asparagine binding pocket. Such modified asparaginyl hydroxylases can then be produced using standard techniques. The expected activity can then be assayed as described in more detail below, for example, to identify whether the hydroxylase activity with respect to HIF has been reduced or removed, or alternatively, to assess the asparaginyl activity or binding in respect to other substrates.

Compounds which have been identified in accordance with the present invention can be further analysed in assays to monitor for activity of the asparagine hydroxylase enzyme directly. Agents which inhibit or reduce HIF asparagine hydroxylase activity reduce hydroxylation of HIF-α and lead to an increase in the interaction with P300 and in particular the CH1 domain and thus transcriptional activation. This in turn will lead to the activation of systemic local defences against

hypoxia or ischaemia that may include the promotion of angiogenesis, erythropoesis, energy metabolism, inflammation, vasomotor function and will also affect apoptotic/proliferative responses.

We describe below in more detail a number of different assays that may be carried out to assay the activity of modulators of HIF hydroxylase activity or of FIH identified in accordance with the present invention and in particular of asparagine hydroxylase activity, or which affect regulation of HIF-α interaction with p300 in a cell and hence which affect HIF mediated activity. Some of these assays utilise HIF polypeptides, and HIF asparagine hydroxylases. Typically, the assays may utilise a human HIF asparagine hydroxylase such as FIH or a fragment or variant of a human HIF asparagine hydroxylase. These components are described in more detail below. Each of these components, where required, may be provided either in purified or unpurified form, for example, as cellular extracts or by purification of the relevant component from such extracts. Alternatively, the relevant component can be expressed using recombinant expression techniques and purified for use in the assay. Alternatively, the components may be expressed recombinantly in a cell for use in cell based assays.

Typically, a polynucleotide encoding the relevant component is provided within an expression vector. Such expression vectors are routinely constructed in the art and may for example involve the use of plasmid DNA and appropriate initiators, promoters, enhancers and other elements, such as for example polyadenylation signals which may be necessary and which are positioned in the correct orientation in order to allow full protein expression. Suitable vectors would be very readily apparent to those of skill in the art, such as those described in more detail herein with reference to the HIF hydroxylases. Promoter sequences may be inducible or constitutive promoters depending on the selected assay format. The promoter may be tissue specific. Examples of promoters and other flanking sequences for use in the expression vectors are described in more detail herein with reference to the HIF hydroxylases of the invention and in particular to the human HIF hydroxylases.

HIF Polypeptides and Peptide Analogues

The assays of the present invention may use a substrate of a HIF asparagine hydroxylase and in particular an asparagine containing substrate of the enzyme. In particular, such substrates may be used in assays to monitor for the activity of a modulator of HIF asparagine hydroxylase activity. The substrate may be a HIF polypeptide or peptide analogue thereof. Typically, a HIF polypeptide will be used as the substrate.

Any suitable substrate in which an asparagine residue is hydroxylated by a FIH may be used. In preferred embodiments of the invention, such a substrate is a HIF polypeptide such as a HIF-1α or HIF-2α subunit protein or fragment of either or peptide analogue of the subunit or fragment. Preferably, the HIF-α peptide conveys an oxygen regulated response. Preferably, the HIF-α peptide has a CAD domain and is capable of oxygen regulated interaction with p300 and downstream transcriptional activation. Preferably, such HIF-α peptides are capable of interacting with the p300 CH1 domain. Preferably, such HIF polypeptides, fragments or peptide analogues incorporate an asparagine residue equivalent to Asn 803 defined with reference to HIF-1α. The asparagine equivalent to Asn 803 of HIF-1α may be determined by aligning the HIF variant, fragment or analogue to the sequence of HIF-1α to obtain the best sequence alignment and identifying thereby the asparagine equivalent to Asn 803 of HIF-1α.

A HIF polypeptide may be of eukaryotic origin, in particular a human or other mammalian, HIF-α subunit protein or fragment thereof. Alternatively, the polypeptide may be of *C. elegans* origin. In those assays which monitor for hydroxylation of HIF-α through its interaction with p300, the HIF polypeptide has the ability to bind to a wild type full length p300 protein or a fragment thereof comprising the CH1 domain. Preferably, such binding is able, in a hypoxic cellular environment, to activate transcription.

A number of HIFα subunit proteins have been cloned. These include HIF-1α, the sequence of which is available as Genbank accession number U22431, HIF-2α, available as Genbank accession number U81984 and HIF-3α, available as Genbank accession numbers AC007193 and AC079154. These are all human HIF α subunit proteins and all may be used in the invention. HIF-α subunit proteins from

other species, including murine HIF-1α (accession numbers AF003695, U59496 and X95580), rat HIF-1α (accession number Y09507), murine HIF-2α (accession numbers U81983 and D89787) and murine HIF-3α (accession number AF060194) may also be used in the invention.

One HIF-α protein of particular interest is the *C.elegans* HIF-α subunit protein. The *C.elegans* system may be used in assays of the present invention.

There are a number of common structural features found in the two HIF-α subunit proteins identified to date. Some of these features are identified in O'Rourke *et al* (1999, J. Biol. Chem., 274; 2060-2071) and may be involved in the trans-activation functions of the HIF-α subunit proteins. One or more of these common structural features are preferred features of the HIF polypeptides.

Variants of the above HIF-α subunits may be used, such as synthetic variants which have at least 45% amino acid identity to a naturally occurring HIF-α subunit (particularly to a human HIF-α subunit such as, for example HIF-1α), preferably at least 50%, 60%, 70%, 80%, 90%, 95% or 98% identity. Such variants may include substitutions or modifications as described above with respect to HIF hydroxylases. Amino acid activity may also be calculated as described above with reference to HIF hydroxylases.

HIF fragments may also include non-peptidyl functionalities and may be optimised for assay purposes such that the level of identity is lowered. Such functionalities may be covalently bound such as sugars or non-covalently bound such as metal ions.

HIFα polypeptides as described herein may be fragments of the HIF-α subunit protein or variants as described above, provided that said fragments retain the ability to interact with a wild-type p300 CH1 domain. When using proteinogenic amino acid residues, such fragments are desirably at least 20, preferably at least 40, 50, 75, 100, 200, 250 or 400 amino acids in size. Desirably, such fragments include asparagine 803.

Cell based assays of the present invention may involve upregulation of an endogenous HIF-α or expression of a HIF-α by recombinant techniques and in particular of HIF-1α.

Assay Methods

The present invention provides an assay method for an agent identified as a modulator of asparagine hydroxylation of hypoxia inducible factor. The method comprises contacting a HIF asparagine hydroxylase and a test substance in the presence of a substrate of the hydroxylase under conditions in which asparagine hydroxylation occurs in the absence of the test substrate and determining asparagine hydroxylation of the substrate. In an alternative assay, HIF asparagine hydroxylase and the test substance are contacted in the presence of the substrate of the hydroxylase under conditions in which hydroxylation does not occur in the absence of the test substrate. Determination of any asparagine hydroxylation is monitored to identify whether the agent actively acts as a promoter of asparagine hydroxylase.

FIH has been found to hydroxylate HIF-α at an asparagine residue within the CAD domain. This hydroxylation mediates p300 binding and in particular, reduces p300 binding. Such binding leads to transcriptional activation. This interaction and activation may also be used as the basis for an assay of the invention.

Such assays of the present invention may be used to assay the activity of inhibitors of HIF asparagine hydroxylase activity and are thus preferably carried out under conditions under which asparagine hydroxylation would take place in the absence of the test substance. The assays of the invention may also be used to assay the activity of inhibitors which are specific for HIF asparagine hydroxylases and which do not have activity or are less active with other hydroxylases, for example, such as HIF prolyl hydroxylases or other asparagine/aspartamic acid hydroxylases. The assays of the invention may also be used to assay the activity of hydroxylase modulators, such as HIF prolyl hydroxylase inhibitors which are not expected to have activity on FIH based on structural modelling studies, and hence may be used to identify inhibitors which are specific for prolyl hydroxylase.

Methods for monitoring modulation

The precise format of any of the screening or assay methods of the present invention may be varied by those of skill in the art using routine skill and knowledge. The skilled person is well aware of the need to additionally employ appropriate controlled experiments. The assays of the present invention may involve monitoring

for asparagine hydroxylation of a suitable substrate, monitoring for the utilisation of substrates and co-substrates, monitoring for the production of the expected products between the enzyme and its substrate. Assay methods of the present invention may also involve screening for the direct interaction between components in the system. Alternatively, assays may be carried out which monitor for downstream effects such as binding of HIF by p300 and downstream effects mediated by HIF such as HIF mediated transcription using suitable reporter constructs or by monitoring for the upregulation of genes or alterations in the expression patterns of genes know to be regulated directly or indirectly by HIF.

Various methods for determining hydroxylation are known in the art and are described and exemplified herein. Any suitable method may be used for determining activity of the HIF hydroxylase such as by substrate or co-substrate utilization, product appearance such as peptide hydroxylation or down-stream effects mediated by hydroxylated or non-hydroxylated products.

Assays may be carried out to monitor directly for hydroxylation of the relevant asparagine residue or another position. Alternatively, assays may be carried out to monitor for depletion of co-factors and co-substrates. Alternatively, such assays may monitor the downstream effects of hydroxylation of HIF or indeed inhibition of hydroxylation of HIF, for example, by monitoring the interaction between HIF and p300 or HIF mediated transcription. Alternatively, reporter gene constructs driven by HIF regulated promoters may be used. Assays are also provided for the identification of enhancers of the activity of the HIF asparagine hydroxylase. Such enhancers may be used to reduce HIFα activity.

In one embodiment, a suitable substrate of the HIF asparagine hydroxylase is provided. This may be HIF-α or a fragment thereof which includes a CAD domain or which includes a residue equivalent to Asn 803 of HIF-1α. The substrate may not be initially hydroxylated at the Asn 803 position. This may be achieved by providing synthetic polypeptide substrates, or by producing HIF-α polypeptides in bacterial cells, insect cells or mammalian cells or in *in vitro* transcription and translation systems. Alternatively, assays may be carried out over a selected time course such that the substrate is produced during the course of the assay, initially in un-hydroxylated form.

The substrate, enzyme and potential inhibitor compound may be incubated together under conditions which, in the absence of inhibitor provide for hydroxylation of Asn 803, and the effect of the inhibitor may be determined by determining hydroxylation of the substrate. This may be accomplished by any suitable means. Small polypeptide substrates may be recovered and subject to physical analysis, such as mass spectrometry or chromatography, or to functional analysis, such as the ability to bind to p300 (or displace a reporter molecule from p300). Such methods are known as such in the art and may be practiced using routine skill and knowledge. Determination may be quantitative or qualitative. In both cases, but particularly in the latter, qualitative determination may be carried out in comparison to a suitable control, e.g. a substrate incubated without the potential inhibitor.

Inhibitor compounds which are identified in this manner may be recovered and formulated as pharmaceutical compositions.

Assays in accordance with the present invention may involve monitoring for the interaction between p300 and HIF. The interaction between HIF and p300 is mediated by hydroxylation of HIF. Transcription and expression of genes known to be upregulated or down regulated by the presence of HIF could be monitored. In particular, upregulation of HIF regulated genes would demonstrate inhibition of asparagine hydroxylation whereas down regulation would suggest enhancement or promotion of asparagine hydroxylation.

In alternative embodiments, reporter constructs may be provided in which promoters mediated by HIF are provided operably linked to a reporter gene. Any suitable reporter gene could be used, such as for example enzymes which may then be used in colorometric, fluorometric, fluorescence resonance or spectrometric assays.

HIF asparagine hydroxlase is a 2OG dependent oxygenase. In the assay methods described herein, typically the HIF asparagine hydroxylase and the substrate of the hydroxylase are contacted in the presence of a co-substrate, such as 2-oxoglutarate (2OG). The hydroxylase activity of the HIF hydroxylase may be determined by determining the turnover of the co-substrate. This may be achieved by determining the presence and/or amount of reaction products, such as hydroxylated

substrate or succinic acid. The amount of product may be determined relative to the amount of substrate. Typically, in such embodiments the substrate may be an HIF-α polypeptide and, for example, the product measured may be hydroxylated HIF-α polypeptide.

Alternatively, the end-point determination may be based on conversion of HIFα or peptide fragments (including synthetic and recombinant peptides) derived from HIFα into detectable products. Peptides may be modified to facilitate the assays so that they can be rapidly carried out and may be suitable for high throughput screening.

For example, reverse phase HPLC (C-18 octadecylsilane column), may be used to separate starting synthetic peptide substrates for HIF hydroxylase from the asparagine hydroxylated products, as the latter have a shorter retention time in the column. Modifications of this assay or alternative assays for HIF hydroxylase activity may employ, for example, mass spectrometric, spectroscopic, and/or fluorescence techniques as are well known in the art (Masimirembwa C. *et al* Combinatorial Chemistry & High Throughput Screening (2001) 4 (3) 245-263, Owicki J. (2000) J. Biomol. Screen. 5 (5) 297-305, Gershkovich A *et al* (1996) J. Biochem. & Biophys. Meths. 33 (3) 135-162, Kraaft G. *et al* (1994) Meths. Enzymol. 241 70-86). Fluorescent techniques may employ versions of the substrate modified in such as way as to carry out or optimise spectroscopic or fluorescence assays.

For example, HIFα polypeptide may be immobilised e.g. on a bead or plate, and hydroxylation of the appropriate residue detected using an antibody or other binding molecule which binds the CAD binding domain of HIFα with a different affinity when an asparagine 803 is hydroxylated from when the residue is not hydroxylated. Such antibodies may be obtained by means of standard techniques which are well known in the art, e.g. using a hydroxylated HIFα peptide.

Binding of a molecule which discriminates between the hydroxylated and non-hydroxylated form of a HIFα polypeptide may be assessed using any technique available to those skilled in the art, which may involve determination of the presence of a suitable label.

Assay methods of the present invention may also take the form of an *in vivo* assay. The *in vivo* assay may be performed in a cell line such as a yeast strain in which the relevant polypeptides or peptides are expressed from one or more vectors introduced into the cell.

5

In vivo assays

The assays may be carried out using cell based, organ based or whole animal assays conducted *in vivo*. Such assays may utilize the endogenous expression of the HIF hydroxylase nucleotides and/or polypeptides. In other forms of the invention, 10 upregulation of specific endogenous HIF hydroxylases may be achieved by stimulators of the expression thereof. Such stimulators may be growth factors or chemicals that upregulate specific HIF asparagine hydroxylases. In another form of the assay, nucleotide constructs may be introduced into cells or transgenic animals to increase production of one or more specific HIF asparagine hydroxylases.

15 HIF complexed with p300 activate hypoxia response elements that are found in the promoters and/or enhancers of endogenous genes that are regulated by the said HIF complexes. Such hypoxia response elements may also be isolated and operationally linked to reporter genes so as to assay the activity of the HIF complex through detection and/or quantitation of the reporter gene or its product. Therefore in 20 a further form of the invention the activity of a HIF-α polypeptide that is regulated by HIF asparagine hydroxylase will be assayed by measuring the effects of the HIF complex on the expression of an endogenous gene or reporter gene that is functionally linked to a HIF binding hypoxia response element. Examples of endogenous genes that are regulated in this way are to be found in the role of the aryl 25 hydrocarbon nuclear translocator (ARNT) in hypoxic induction of gene expression, see for example, Studies in ARNT-deficient cells. S.M. Wood, J.M. Gleadle, C.W. Pugh, O. Hankinson, P.J. Ratcliffe. Journal of Biological Chemistry 271 (1996) 15117-15123, and Hypoxia inducible expression of tumor-associated carbonic anyhydrases, C.C. Wykoff, N.J.P. Beasley, K.J. Turner, J. Pastorek, A. Sibtain. G.D. 30 Wilson, H. Turley, K. Talks, P.H. Maxwell, C.W. Pugh, P.J. Ratcliffe, A.L. Harris. Cancer Research 60 (2000) 7075-7083. Examples include but are not limited to glucose transporter isoform 1, phosphoglycerate kinase-1, carbon anhydrase isoform

9, vascular endothelial growth factor. Each of said genes contains one or hypoxia response elements that may be isolated and operationally linked as single or multiple copies to a reporter gene for the measurement of activity of a HIF-α polypeptide that varies in accordance with the activity of a HIF hydroxylase.

The activity of genes or gene products that are regulated by a HIF-α polypeptide in accordance with the activity of a HIF hydroxylase affects cellular, organ, and animal physiology. Assays that utilise a specific functional response that is regulated in accordance with the activity of a HIF-α polypeptide in accordance with the activity of a HIF hydroxylase may be used. Such responses include the uptake rate of glucose or glucose analogues that are not metabolized, the growth of blood vessels by angiogenesis, the activity of a carbonic anhydrase enzyme. It is recognised that many other responses that operate at a cellular or systemic level are controlled by the activity of a HIF-α polypeptide in accordance with the activity of a HIF hydroxylase and may be utilized as assays of the said HIF hydroxylase activity in further aspects of the invention.

A HIF-α polypeptide that is a substrate for a HIF hydroxylase may be fused to a further polypeptide so as to cause the activity of the said HIF hydroxylase to regulate the activity of the fusion peptide. Accordingly a further form of the invention provides for the assay of the activity of a fusion polypeptide. In the preferred form such a fusion polypeptide may contain the whole of part of a HIF-α polypeptide, particularly including Asn 803, or the CAD domain. The Gal4 DNA binding domain including the amino acids 1-143 together with the Gal binding upstream activating sequence (UAS) is an example of such a transcription factor and cognate DNA response element whose operation can be assayed by those skilled in the art.

Selectivity

It may also be advantageous to modulate HIF asparagine hydroxylase selectively, as a single target, or in selected hydroxylase groups as well as an entire family. Agents which modulate HIF asparagine hydroxylase activity are therefore preferably specific i.e. they have an increased or enhanced effect on a HIF asparagine hydroxylase relative to other 2OG dependent oxygenases.

Assay methods as described herein may therefore further comprise contacting the test compound with one or more 2OG dependent oxygenases under conditions in which said 2OG dependent oxygenases are normally active and determining activity of said oxygenases. A difference in activity in the presence relative to the absence of test compound is indicative of the test compound modulating the activity of the one or more 2OG dependent oxygenases.

A test compound which provides increased or enhanced modulation of a HIF asparagine hydroxylase, relative to the one or more 2OG dependent oxygenases shows selectivity or specificity for the HIF hydroxylase.

2OG dependent oxygenases may include for example, clavaminte synthase, Alk B deacetoxycephalosporin C synthase, collagen-prolyl-4-hydroxylase,collagen prolyl-3-hydroxylase, lysyl hydroxylase, aspartyl hydroxylase, phytanoyl coenzyme A hydroxylase or gamma-butyrobetaine hydroxylase. 2OG dependent oxygenases may be mammalian, preferably human polypeptides.

The invention provides for the use of such selective inhibitors of HIF asparagine hydroxylases in the manufacture of a medicament for the treatment of a condition associated with reduced HIF activity.

Therapeutic Applications

A compound, substance or agent which is found to have the ability to affect the hydroxylase activity of a HIF asparagine hydroxylase, or the compounds referred to herein as FIH inhibitors has therapeutic and other potential in a number of contexts. For therapeutic treatment, such a compound may be used in combination with any other active substance, e.g. for anti-tumour therapy another anti-tumour compound or therapy, such as radiotherapy or chemotherapy.

An agent identified using one or more primary screens (e.g. in a cell-free system) as having ability to modulate the HIFα asparagine hydroxylation activity of a HIF hydroxylase may be assessed further using one or more secondary screens. A secondary screen may involve testing for an increase or decrease in the amount of HIF-α or HIF activity, for example as manifest by the level of a HIF target gene or process present in a cell in the presence of the agent relative to the absence of the agent.

A HIF hydroxylase or a HIF polypeptide may be used in therapies which include treatment with full length polypeptides or fragments thereof, or otherwise modified polypeptides (e.g. to enhance stability or ensure targeting, including in conjunction with other active agents such as antibodies. For example, mutation of HIF-1α to replace Asn 803 with another amino acid residue may prevent hydroxylation and thus promote interaction of HIF-α with p300 and stimulate transcriptional activation.

Generally, an agent, compound or substance which is a modulator according to the present invention is provided in an isolated and/or purified form, i.e. substantially pure. This may include being in a composition where it represents at least about 90% active ingredient, more preferably at least about 95%, more preferably at least about 98%. Any such composition may, however, include inert carrier materials or other pharmaceutically and physiologically acceptable excipients, such as those required for correct delivery, release and/or stabilisation of the active agent. Typically, the concentration in such compositions is 0.1 to 50%, generally 0.5 to 20%, especially 1 to 10% by weight based on the weight of the composition. As noted below, a composition according to the present invention may include in addition to an modulator compound as disclosed, one or more other molecules of therapeutic use, such as an anti-tumour agent.

Products obtained by assays of the invention

The invention further provides compounds obtained or identified by methods of the present invention, and compositions comprising said compounds, such as pharmaceutical compositions wherein the compound is in a mixture with a pharmaceutically acceptable carrier or diluent. The carrier may be liquid, e.g. saline, ethanol, glycerol and mixtures thereof, or solid, e.g. in the form of a tablet, or in a semi-solid form such as a gel formulated as a depot formulation or in a transdermally administerable vehicle, such as a transdermal patch.

The invention further provides a method of treatment which includes administering to a patient an agent which interferes with the hydroxylation of the asparagine target residue of an HIFα polypeptide by a HIF hydroxylase. Such agents may include inhibitors of asparagine hydroxylase activity. The invention also

provides a method of treatment which includes administering to a patient a compound as defined above.

The therapeutic/prophylactic purpose may be related to the treatment of a condition associated with reduced or suboptimal or increased HIF levels or activity, or conditions in which have normal HIF levels, but where an modulation in HIF activity such as an increase or decrease in HIF activity is desirable such as:

(i) ischaemic conditions, for example organ ischaemia, including coronary, cerebrovascular and peripheral vascular insufficiency. The therapy may be applied in two ways; following declared tissue damage, e.g. myocardial infarction (in order to limit tissue damage), or prophylactically to prevent ischaemia, e.g. promotion of coronary collaterals in the treatment of angina.

(ii) wound healing and organ regeneration

(iii) auto-, allo-, and xeno- transplantation.

(iv) systemic blood pressure

(v) cancer; HIFα is commonly up-regulated in tumour cells and has major effects on tumour growth and angiogenesis.

(vi) inflammatory disorders.

(vii) pulmonary arterial blood pressure, neurodegenerative disease.

Modulating HIF prolyl hydroxylase activity in a person, an organ, or a group of cells may be exploited in different ways to obtain a therapeutic benefit:

(a) Non cell autonomous: The HIF system is used by cells to influence the production of substances which signal to other cells. These signals may then have effects at (i) a distant site (for example erythropoietin acts on the bone marrow) or (ii) locally (angiogenic growth factors increase the local formation of blood vessels). Manipulating non cell autonomous behaviour via altering hydroxylase activity is therefore useful in the treatment of anaemia, and local ischaemia, for example in the eye, brain, heart and limbs. Many other signals that are involved in aspects of physiological homeostasis may be, or are known to be, adjusted by HIF activation. Consequently altering HIF prolyl hydroxylase activity may be used to potentiate or initiate a helpful response for a therapeutic benefit, or to prevent or ameliorate a harmful response. For example, this approach can be used to alter appetite, or blood pressure in the systemic or pulmonary beds.

(b) Cell autonomous: the HIF system is also used by cells to regulate cellular metabolism, and decisions concerning differentiation, proliferation and apoptosis. Therefore manipulating the HIF system can be used to alter the viability and behaviour of cells. An increase in cell viability can be achieved by increasing HIF activation, for example in an ischaemic tissue. This approach can also be used in improving pancreatic beta cell viability as a way of ameliorating diabetes, or of improving the viability or function of a group or groups of neurons in Parkinson's disease, motorneurone disease or forms of dementia. In a different approach, the HIF signal can be manipulated to prevent a group of cells proliferating, or to promote its death or differentiation. For example transient activation of the HIF system in a malignant tumour can be used to provoke death of a substantial number of tumour cells.

Pharmaceutical Compositions

In various further aspects, the present invention thus provides a pharmaceutical composition, medicament, drug or other composition for such a purpose, the composition comprising one or more agents, compounds or substances as described herein, including HIF asparagine hydroxylase inhibitors, or one or more compounds of formula (A) to (F) or derivatives thereof, the use of such a composition in a method of medical treatment, a method comprising administration of such a composition to a patient, e.g. for treatment(which may include preventative treatment) of a medical condition as described above, use of such an agent compound or substance in the manufacture of a composition, medicament or drug for administration for any such purpose, e.g. for treatment of a condition as described herein, and a method of making a pharmaceutical composition comprising admixing such an agent, compound or substance with a pharmaceutically acceptable excipient, vehicle or carrier, and optionally other ingredients.

In one embodiment the method for providing a pharmaceutical composition may typically comprise:

(a) identifying an agent in accordance with the invention; and

(b) formulating the agent thus identified with a pharmaceutically acceptable excipient.

The agent may be used as sole active agent or in combination with one another or with any other active substance, e.g. for anti-tumour therapy another anti-tumour compound or therapy, such as radiotherapy or chemotherapy.

Whatever the agent used in a method of medical treatment of the present invention, administration is preferably in a "prophylactically effective amount" or a "therapeutically effective amount" (as the case may be, although prophylaxis may be considered therapy), this being sufficient to show benefit to the individual. The actual amount administered, and rate and time-course of administration, will depend on the nature and severity of what is being treated. Prescription of treatment, e.g. decisions on dosage etc, is within the responsibility of general practitioners and other medical doctors.

An agent or composition may be administered alone or in combination with other treatments, either simultaneously or sequentially dependent upon the condition to be treated, e.g. as described above.

Pharmaceutical compositions according to the present invention, and for use in accordance with the present invention, may include, in addition to active ingredient, a pharmaceutically acceptable excipient, carrier, buffer, stabiliser or other materials well known to those skilled in the art. In particular they may include a pharmaceutically acceptable excipient. Such materials should be non-toxic and should not interfere with the efficacy of the active ingredient. The precise nature of the carrier or other material will depend on the route of administration, which may be oral, or by injection, e.g. cutaneous, subcutaneous or intravenous. The compositions will typically be sterile.

Pharmaceutical compositions for oral administration may be in tablet, capsule, powder or liquid form. A tablet may include a solid carrier such as gelatin or an adjuvant. Liquid pharmaceutical compositions generally include a liquid carrier such as water, petroleum, animal or vegetable oils, mineral oil or synthetic oil. Physiological saline solution, dextrose or other saccharide solution or glycols such as ethylene glycol, propylene glycol or polyethylene glycol may be included.

For intravenous, cutaneous or subcutaneous injection, or injection at the site of affliction, the active ingredient will be in the form of a parenterally acceptable aqueous solution which is pyrogen-free and has suitable pH, isotonicity and stability.

Those of relevant skill in the art are well able to prepare suitable solutions using, for example, isotonic vehicles such as Sodium Chloride Injection, Ringer's Injection, Lactated Ringer's Injection. Preservatives, stabilisers, buffers, antioxidants and/or other additives may be included, as required.

Liposomes, particularly cationic liposomes, may be used in carrier formulations. Examples of techniques and protocols mentioned above can be found in Remington's Pharmaceutical Sciences, 16th edition, Osol, A. (ed), 1980.

The substance or composition may be administered in a localised manner to a particular site or may be delivered in a manner in which it targets particular cells or tissues, for example using intra-arterial stent based delivery.

Targeting therapies may be used to deliver the active substance more specifically to certain types of cell, by the use of targeting systems such as antibody or cell specific ligands. Targeting may be desirable for a variety of reasons, for example if the agent is unacceptably toxic, or if it would otherwise require too high a dosage, or if it would not otherwise be able to enter the target cells.

In a further embodiment the invention provides for the use of an agent of the invention in the manufacture of a medicament for the treatment of a condition associated with increased or decreased HIF levels or activity. The condition may, for example, be selected from the group consisting of ischaemia, wound healing, auto-. allo-, and xeno- transplantation, systemic high blood pressure, cancer, and inflammatory disorders.

Examples

**Example 1**

The position on Asn803 of human HIF-1α that is hydroxylated was identified as described in the following. cDNA sequences encoding FIH-1 were cloned into the pET28a(+) vector (from Novagen) to yield FIH-1 protein with an N-terminal $His_6$tag to facilitate purification. Purification of crude material by nickel affinity chromatography, followed by thrombin cleavage of the $His_6$ tag, and size exclusion chromatography (Superdex S75) yielded >95% pure protein by SDS-PAGE analysis. Mass spectrometry confirmed the identity of the isolated species. The 19-residue

peptide comprising amino acids 788-806 of human HIF-1α was modified by aerobic incubation with FIH-1 FIH (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002) in the presence of ascorbate, DTT, catalase, 2-oxoglutarate, and iron(II) for 30 minutes at 37°C. The reaction was quenched by cooling to 4°C and addition of an equal volume of methanol. Precipitate was removed by centrifugation and the supernatant purified by HPLC using a Jupiter C4 column (15cm x 4.6mm). Peptide was eluted using a gradient of acetonitrile in 0.1% trifluoroacetic acid, freeze-dried from the HPLC solvent for amino acid and mass spectrometric analyses. The sample was freeze-dried a second time from $D_2O$ in preparation for NMR analysis.

Catalytic FIH-1 mediated hydroxylation of a synthetic 19 residue peptide corresponding to residues 788-806 of HIF-1α was confirmed by mass spectrometric analysis of HPLC purified material: Native peptide 19mer $[M+2H]^{2+}$ = 1026.67Da, modified peptide 19mer $[M+2H]^{2+}$ = 1034.61Da, a mass difference of +8Da of the doubly charged ions, corresponding to +16Da in the peptide (oxygen). N-Terminal Edman degradation of the product peptide gave the following sequence: DESGLPQLTSYDCEVxA, where x was not asparagine. The peak from this (16th) cycle of Edman degradation ran to a similar position as the β-hydroxyasparagine standard. Acid hydrolysis of the modified peptide followed by amino acid analysis showed the presence of β-hydroxyaspartic acid only.

Both $^{1}H$ and $^{13}C$ chemical shift changes between the 19mer peptide substrate and the HPLC purified incubation product were assessed by 2D $^{1}H$-$^{13}C$ HSQC experiments. In the substrate a grouping of four β-$CH_2$ resonances were assigned as belonging to Asp-1, Tyr-11, Asp-12 and Asn-16 according to their $^{1}H$ and $^{13}C$ shifts (Evans, J. N. S. (1995) Biomolecular NMR Spectroscopy, Oxford University Press, Oxford, UK). In the product it was clear from both the 2D HSQC and the 1D proton spectra that only three of these four resonances are present. Comparison of the two spectra indicates that the signal assigned to the Asn-16 β-carbon (at δH 2.813 and 2.695ppm and δC 37.40ppm in the substrate) has disappeared, consistent with hydroxylation of the asparagine residue at its β-carbon. The resonances due to the two aspartic acid residues had shifted slightly, presumably due to changes in the protonation state, and now occur at a similar $^{1}H$ chemical shift as the β-protons of the

asparagine in the substrate. A difference in the oxidation state of the cysteine between the two samples in unlikely given the near identical chemical shifts for the cysteinyl β-carbon and hydrogens. The change from a double doublet to a single doublet for the β-hydrogen of the hydroxylated residue also rules out any possibility the observed alterations in the NMR spectrum are due to aggregation. Two new resonances have appeared in the product spectrum at δH 4.913 ppm and δC 56.26 ppm and at δH 4.654 ppm and δC 72.22 ppm. These resonances correlate with one another in the 2D COSY spectrum and share a $^{1}H$-$^{1}H$ coupling constant of 2.4 Hz and are therefore assigned as the $CH^{\alpha}$-$CH^{\beta}$ of the hydroxylated asparagine. The appearance of these resonances also coincides with the disappearance of the δH 4.706 ppm and δC 51.43 ppm resonances observed in the substrate spectra, which is therefore assigned as the $CH^{\alpha}$ of the parent asparagine prior to modification. Comparison of the $CH^{\alpha}$-$CH^{\beta}$ coupling constant of 2.4Hz observed for the hydroxylated Asn-803, with literature values implied the *threo* isomer is produced.

In summary of the above 'NMR experiments: The HSQC experiments gave direct evidence for hydroxylation occurring at the β-carbon of the target asparagine, with the hydroxylated β-carbon appearing significantly deshielded (at 72.22 ppm) and the adjacent α-carbon deshielded to a lesser extent (at 56.26 ppm) relative to the parent asparagine. Changes of these magnitudes in the $^{13}C$ chemical shifts are inconsistent with hydroxylation of the side-chain nitrogen, but consistent with hydroxylation at the β-carbon. Further, the $^{13}C$ spectrum of free DL-*threo*-β-hydroxyasparagine (this study), has resonances at 58.63ppm and 73.85ppm corresponding to α- and β-carbons. The product assignment is also consistent with $^{1}H$-NMR chemical shifts of the α- and β-hydrogens in the β-hydroxyaspartyl residues in EGF-like domains which are 4.48ppm and 4.36ppm respectively (with respect to water at 4.75ppm) when calcium is absent (Selander et al, Biochemistry **29**, 8111-8118). The analysis of the coupling constant reported here suggests that the *threo*-isomer is the one formed on hydroxylation of Asn-803 by FIH-1.

Two reports (Dames et al., (2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 52715276; Freedman et al, (2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 53675372) reveal how β-hydroxylation of Asn-803 of HIF-1α would be damaging to complex formation with

p300. Although the position of hydroxylation was not identified in either report, both imply that hydroxylation at the *pro-S* position of the β-carbon, *i.e.* to give the *threo (2S, 3S)*-isomer, would interfere with the hydrogen bonding that maintains the α-helical conformation adopted by this part of HIF-1α, and also create a need for the energetically unfavourable desolvation of the hydroxyl group. A steric clash between the inserted *pro-S* hydroxyl group and Ile-353 (numbering from Dames *et a l*(2002) *Proc. Natl. Acad. Sci. U. S. A.* **99**, 52715276) of p300 would disrupt the interaction of the two proteins. Presumably the same mechanism is also used to abrogate the interaction of HIF-2α and p300. The discovery that it is the beta-position of Asn-803 that is modified and the associated mechanistic implications may be used in the design of compounds that bind to p300 thereby displacing HIF-alpha and/in the design of inhibitors of FIH (see below); in both cases to enable pro-angiogenetic pharmaceutical agents.

**Example 2**

To obtain an FIH:CAD complex suitable for X-ray analysis without oxidation of the CAD or the $Fe^{(II)}$, FIH and various CAD fragments from seven to fifty-two residues were co-crystallised with $Fe^{(II)}$ and 2OG under anaerobic conditions. Structures were also obtained for FIH complexed with $Fe^{(II)}$ and *N*-oxaloylglycine (NOG, an FIH inhibitor), (anaerobically) and $Zn^{(II)}$ and NOG (aerobically). These structures were solved by molecular replacement using a model obtained by multiple anomalous dispersion on selenomethionine-substituted apo-FIH. Crystalline FIH:CAD complexes were obtained with $CAD_{786-826}$, $Fe^{(II)}$ and NOG or 2OG (structures 1 and 2, Table 1), $CAD_{775-826}$ with $Zn^{(II)}$ and NOG (structure 3). Crystallisation attempts with $CAD_{787-806}$, $CAD_{850-862}$ (HIF-2α, equivalent to HIF-1α $CAD_{802-814}$) and $CAD_{800-806}$ did not result in FIH:CAD complexes; solution analyses indicated that CAD fragments shorter than twenty resides are not efficient *in vitro* substrates.

**Table 1 Summary of FIH:CAD-fragment complex structures***

| Structure No. | Resolution (Å) | Metal | Co-substrate | Co-crystallisation CAD peptide | Site 1 CAD residues resolved | Site 2 CAD residue resolved | $R_{free}$ (%) | R.m.s.d. from Struct. 1 (Å) | PDB ID. |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.15 | Fe | NOG | HIF-1α 786-826 | 795-806 | 812-823 | 21.3 | - | 1H2K |
| 2 | 2.25 | Fe | 2OG | HIF-1α 786-826 | 795-806 | 813-822 | 21.7 | 0.149 | 1H2L |
| 3 | 2.50 | Zn | NOG | HIF-1α 775-826 | 795-806 | 813-822 | 22.5 | 0.136 | 1H2M |
| 4 | 2.84 | Fe | 2OG | HIF-2α 850-862 | - | - | 25.7 | 0.226 | 1H2N |

*Crystalline FIH:CAD complexes were also obtained with $Fe^{(II)}$, HIF-1α 775-786 and 2OG or NOG.

Methods employed in structural work

Protein expression, purification and crystallisation

FIH, $CAD_{775-826}$ and $CAD_{786-826}$ were prepared as described (Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). Selenomethionine (SeMet) substituted FIH was produced using a metabolic inhibition protocol and LeMaster media supplemented with 50 mg/l L-selenomethionine. SeMet incorporation was >95 % by ESI-MS. Aerobic crystallisation of SeMet FIH (at 11 mg $ml^{-1}$) was accomplished by hanging-drop vapour diffusion at 17 °C. The mother liquor consisted of 1.2 M ammonium sulphate, 4 % PEG 400 and 0.1 M Hepes pH 7.5. Crystallisation of FIH:Fe:CAD fragment complexes was accomplished under an anaerobic atmosphere of argon in a Belle Technology glove box (0.3-0.4 ppm $O_2$) using the same mother liquor and a solution containing FIH (at 11 mg $ml^{-1}$), $Fe^{2+}$ (1 mM), 2OG/NOG (2 mM) and CAD fragment (1 mM). Crystallisation of FIH:Zn:CAD fragment was accomplished aerobically under similar conditions. Peptides were either synthesised by solid phase peptide synthesis or purchased from Biopeptide Co. (San Diego, USA).

Crystallographic data collection and structure refinement

Crystals were cryocooled by plunging into liquid nitrogen and X-ray data were collected at 100 K using a nitrogen stream. Cryoprotection was accomplished by sequential transfer into a solution containing 1.2 M ammonium sulphate, 3 % PEG 400, 0.1 M Hepes pH 7.5 and 10 % followed by 24 % glycerol. A three-wavelength multiple anomalous dispersion (MAD) dataset was collected to 2.9 Å resolution on beamline 14.2 of the Synchrotron Radiation Source, Daresbury, U.K. Data from crystals of FIH:CAD complexes were collected on beamlines 14.2, 9.6 or 9.5 using ADSC Quantum 4 (14.2 and 9.6) or MarCCD detectors (9.5). All data was processed with the program MOSFLM and the CCP4 suite[Collaborative Computational Project Number 4 *Acta Crystallogr.* **D50**, 760-763 (1994)]. The crystals belonged to space group $P4_12_12$. Six selenium positions were located and phases calculated using the program SOLVE (Terwilliger et al. **D55**, 849-861, 1999). Density modification, which increased the figure of merit from 0.56 to 0.66, was performed using RESOLVE (Terwilliger *Acta Crystallogr.* **D56**, 965-972 2000).

An initial model was built using the program O (Jones et al, *Acta Crystallogr.* **A47**, 110-119, 1991).and refined against the SeMet data (remote wavelength) using the program CNS (Brunger *Acta Crystallogr.* **D54**, 905-921, 1998).. One cycle of simulated annealing followed by grouped *B*-factor refinement brought the $R_{free}$ to 36.2 %. Following further rebuilding and refinement, which brought the $R_{free}$ to 32.3 %, the model was transferred to the 2.15 Å dataset. Rebuilding and refinement using REFMAC5 including addition of Fe, substrate and solvent molecules, and refinement of TLS parameters brought the conventional *R*-factor to 17.8 % and the $R_{free}$ to 21.3 %. The following residues are missing in the current model: 1-15 and 304-306 of FIH, 786-794, 807-811 and 824-826 of the CAD fragment. According to PROCHECK there are no Ramachandran outliers and 90.7 % of residues have most favourable backbone conformations. For the CAD peptide, 77.8% of residues are in the most favourable region with the remaining 22.2 % in additionally allowed regions.

Other structures were solved by molecular replacement using the coordinates from the 2.15 Å data and refinement using REFMAC5. In all structures electron density for the Fe and 2OG/NOG was visible throughout refinement. Significant positive difference electron density was observed between the iron and the CAD Asn803 β-carbon. Since *B*-factor differences between FIH and CAD imply that the CAD is not at 100 % occupancy, this may represent an alternative binding-mode for the 1-carboxylate 2OG in the absence of substrate although it could also be due to a ligating water molecule, again in the absence of substrate.

Overview of FIH structure

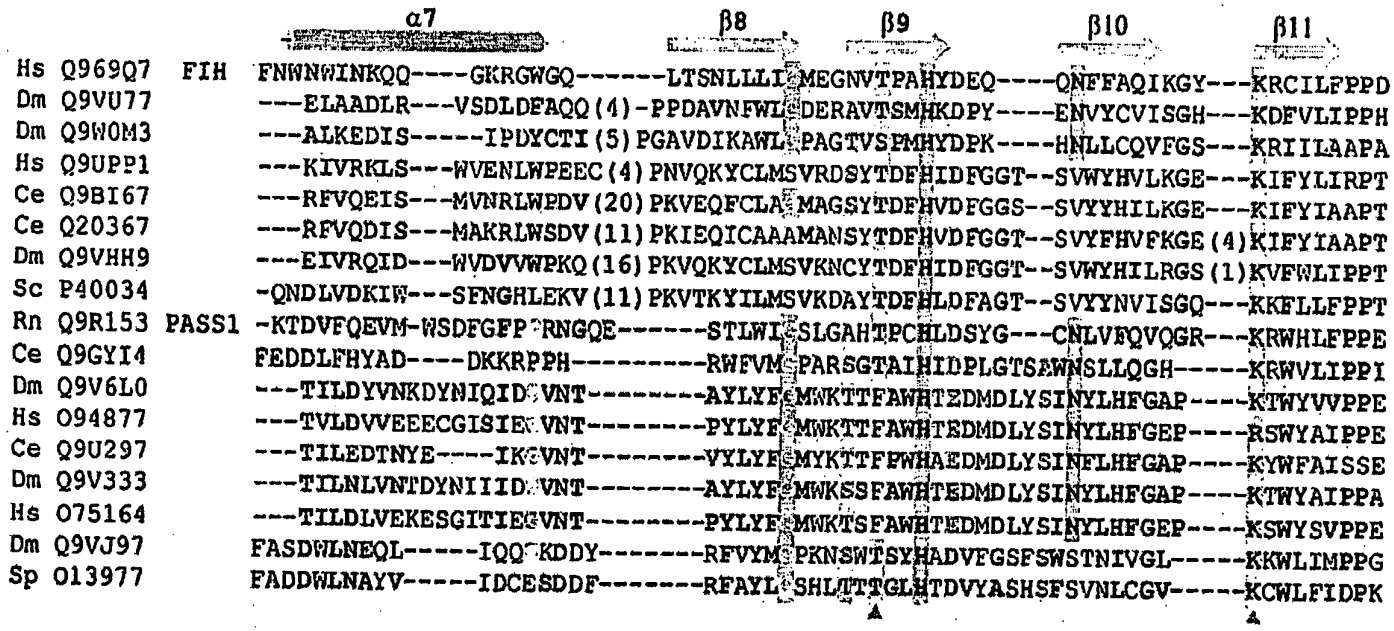
The core of FIH comprises a double-stranded beta-helix (DSBH or jellyroll) motif formed from eight β-strands, β8-β11 and β14-β17. Residues 220-259 form an insert between strands 4 and 5 of the DSBH. The bottom face of the DSBH is flanked by an additional four β-strands from the N-terminal region to form an eight-membered antiparallel β-sheet. The N-terminal strand β1 bisects the face of the DSBH opposite to the active site. The β1 strand has a 360° twist located at a PXXP sequence, in between its interactions with β14 and β2. A similarly positioned β-

strand is found in most 2OG oxygenases, though not always from the same region of the protein. The sheet-helix-sheet motif formed by β1, α1 and β2 is conserved in all enzymes of this class except proline 3-hydroxylase and a similar fold in this region is found in the related $Cu^{(II)}$ utilising quercetin 2,3-dioxygenase (QD) (Fusetti et al, STRUCTURE 10 (2): 259-268 2002). The topology of FIH unequivocally defines it as an iron-binding member of the cupin structural family which already includes QD and $Mn^{(II)}$ utilising Type II phosphomannose isomerase (Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* **26**, 79).

Related enzymes to FIH

FIH has significant sequence similarity with the JmjC homology region of the jumonji transcription factors (Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* **26**, 79; Hewitson et al., J BIOL CHEM 277 (29): 26351-26355, 2002). These proteins are members of the cupin structural superfamily and have been implicated in cell growth and heart development. The 2OG oxygenase iron binding residues had been identified in some JmjC domains but not assigned as an iron binding motif. Sequence searches in the light of the FIH structure reveal many JmjC proteins with conserved residues that include both this motif and others, including FIH residues Lys214 and Thr196 that are unusually involved in binding the 5-carboxylate of 2OG. The structure thus reveals that FIH is a one of a large family of iron and 2OG dependent oxygenases involved in the regulation of transcription. Since some of the assigned JmjC domains other than FIH are associated with diseases and particular phenotypes their (e.g.) inhibition may be of therapeutic value. (See e.g. Hu et al, ONCOGENE 20 (47): 6946-6954 OCT 18 2001 and Clissold, P. M., and Ponting, C. P. (2001) *Trends Biochem. Sci.* **26**, 79 and references therein).

Table 2. Partial sequence alignment of FIH with a selection of JmjC domain containing proteins. FIH secondary structure is indicated above the alignment. Selected 2OG binding residues found in FIH are indicated by dark triangles under the alignment and the two iron binding residues by light triangles. SWALL accession numbers are indicated on the left of the alignment.




Hs = Homo sapiens
Dm = Drosophila melanogaster
Ce = Caenorhabditis elegans
Sc = Saccharomyces cerevisiae
Rn = Rattus norvegicus
Sp = Schizosaccharomyces pombe

FIH = Factor Inhibiting HIF
PASS1 = Protein associating with small stress protein

# TABLE 2

TABLE 3 - Coordinates for structures 1 to 4

Structure 1

Below are the coordinates for structure 1 (the 2.15 Å structure of FIH:Fe(II):NOG:CAD):

```
HEADER    TRANSCRIPTION ACTIVATOR/INHIBITOR       12-AUG-02   1H2K
TITLE     FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE    2 FRAGMENT PEPTIDE
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND   3 CHAIN: A;
COMPND   4 ENGINEERED: YES;
COMPND   5 MOL_ID: 2;
COMPND   6 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND   7 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND   8  MEMBER OF PAS PROTEIN 1;
COMPND   9 CHAIN: S;
COMPND  10 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND  11  RESIDUES 786-826
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   3 ORGANISM_COMMON: HUMAN;
SOURCE   4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE   5 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE   6 EXPRESSION_SYSTEM_PLASMID: PET28A(+);
SOURCE   7 MOL_ID: 2;
SOURCE   8 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   9 ORGANISM_COMMON: HUMAN;
SOURCE  10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE  11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE  12 EXPRESSION_SYSTEM_PLASMID: PGEX-GP-1
KEYWDS    FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
KEYWDS   2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, PHOSPHORYLATION
EXPDTA    X-RAY DIFFRACTION
AUTHOR    J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,I.SCHLEMMINGER,
AUTHOR   2 J.F.SEIBEL,C.J.SCHOFIELD
REVDAT   1   03-SEP-02 1H2K    0
JRNL        AUTH   J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,
JRNL        AUTH 2 I.SCHLEMMINGER,J.F.SEIBEL,C.J.SCHOFIELD
JRNL        TITL   FIH:HIF-FRAGMENT COMPLEXES
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK   2
REMARK   2 RESOLUTION. 2.15 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.0
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) :   2.15
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) :  18.50
REMARK   3   DATA CUTOFF            (SIGMA(F)) : NONE
REMARK   3   COMPLETENESS FOR RANGE        (%) :  99.28
REMARK   3   NUMBER OF REFLECTIONS             :   28171
REMARK   3
```

```
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD          : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION  : RANDOM
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.18026
REMARK   3   R VALUE           (WORKING SET) :  0.17761
REMARK   3   FREE R VALUE                    :  0.21305
REMARK   3   FREE R VALUE TEST SET SIZE   (%) :  7.7
REMARK   3   FREE R VALUE TEST SET COUNT      :  2340
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           :      20
REMARK   3   BIN RESOLUTION RANGE HIGH           :    2.150
REMARK   3   BIN RESOLUTION RANGE LOW            :    2.205
REMARK   3   REFLECTION IN BIN     (WORKING SET) :     1906
REMARK   3   BIN R VALUE           (WORKING SET) :    0.222
REMARK   3   BIN FREE R VALUE SET COUNT          :      152
REMARK   3   BIN FREE R VALUE                    :    0.257
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 2875
REMARK   3   NUCLEIC ACID ATOMS       : 0
REMARK   3   HETEROGEN ATOMS          : 21
REMARK   3   SOLVENT ATOMS            : 194
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) :  25.725
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :    -0.27
REMARK   3    B22 (A**2) :    -0.27
REMARK   3    B33 (A**2) :     0.55
REMARK   3    B12 (A**2) :     0.00
REMARK   3    B13 (A**2) :     0.00
REMARK   3    B23 (A**2) :     0.00
REMARK   3
REMARK   3 ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3  ESU BASED ON R VALUE                                (A): 0.174
REMARK   3  ESU BASED ON FREE R VALUE                           (A): 0.156
REMARK   3  ESU BASED ON MAXIMUM LIKELIHOOD                     (A): 0.147
REMARK   3  ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 5.588
REMARK   3
REMARK   3 CORRELATION COEFFICIENTS.
REMARK   3   CORRELATION COEFFICIENT FO-FC      :   0.961
REMARK   3   CORRELATION COEFFICIENT FO-FC FREE :   0.947
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES     COUNT    RMS     WEIGHT
REMARK   3   BOND LENGTHS REFINED           (A):  2973 ; 0.012 ; 0.021
REMARK   3   BOND LENGTHS OTHERS            (A):  2561 ; 0.001 ; 0.020
REMARK   3   BOND ANGLES REFINED      (DEGREES):  4044 ; 1.374 ; 1.949
REMARK   3   BOND ANGLES OTHERS       (DEGREES):  5979 ; 0.722 ; 3.000
REMARK   3   TORSION ANGLES, PERIOD 1 (DEGREES):   352 ; 4.018 ; 3.000
REMARK   3   TORSION ANGLES, PERIOD 3 (DEGREES):   515 ;17.698 ;15.000
REMARK   3   CHIRAL-CENTER RESTRAINTS    (A**3):   416 ; 0.086 ; 0.200
REMARK   3   GENERAL PLANES REFINED          (A):  3333 ; 0.005 ; 0.020
REMARK   3   GENERAL PLANES OTHERS           (A):   604 ; 0.002 ; 0.020
REMARK   3   NON-BONDED CONTACTS REFINED     (A):   714 ; 0.218 ; 0.300
REMARK   3   NON-BONDED CONTACTS OTHERS      (A):  2499 ; 0.204 ; 0.300
REMARK   3   H-BOND (X...Y) REFINED          (A):   259 ; 0.152 ; 0.500
REMARK   3   H-BOND (X...Y) OTHERS           (A):     4 ; 0.087 ; 0.500
REMARK   3   SYMMETRY VDW REFINED            (A):    18 ; 0.245 ; 0.300
REMARK   3   SYMMETRY VDW OTHERS             (A):    72 ; 0.248 ; 0.300
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REMARK   3   SYMMETRY H-BOND REFINED        (A):    13 ; 0.255 ; 0.500
REMARK   3   SYMMETRY H-BOND OTHERS         (A):     1 ; 0.052 ; 0.500
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS  COUNT   RMS    WEIGHT
REMARK   3   MAIN-CHAIN BOND REFINED    (A**2):  1777 ; 0.618 ; 1.500
REMARK   3   MAIN-CHAIN ANGLE REFINED   (A**2):  2862 ; 1.177 ; 2.000
REMARK   3   SIDE-CHAIN BOND REFINED    (A**2):  1196 ; 1.812 ; 3.000
REMARK   3   SIDE-CHAIN ANGLE REFINED   (A**2):  1182 ; 3.002 ; 4.500
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF NCS GROUPS : NULL
REMARK   3
REMARK   3  TLS DETAILS
REMARK   3   NUMBER OF TLS GROUPS  :    1
REMARK   3
REMARK   3   TLS GROUP :     1
REMARK   3    NUMBER OF COMPONENTS GROUP :    2
REMARK   3    COMPONENTS        C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :   A    15        A   451
REMARK   3    RESIDUE RANGE :   S   795        S   823
REMARK   3    ORIGIN FOR THE GROUP (A):  21.6620  27.4620  28.2370
REMARK   3    T TENSOR
REMARK   3      T11:   0.1474 T22:   0.0149
REMARK   3      T33:   0.0919 T12:  -0.0099
REMARK   3      T13:  -0.0455 T23:   0.0363
REMARK   3    L TENSOR
REMARK   3      L11:   1.0098 L22:   2.2577
REMARK   3      L33:   1.2037 L12:   0.6963
REMARK   3      L13:   0.4840 L23:   1.0420
REMARK   3    S TENSOR
REMARK   3      S11:   0.0288 S12:  -0.1525 S13:  -0.0400
REMARK   3      S21:   0.1459 S22:   0.0002 S23:   0.1021
REMARK   3      S31:   0.1876 S32:  -0.0468 S33:  -0.0290
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED : BABINET MODEL WITH MASK
REMARK   3   PARAMETERS FOR MASK CALCULATION
REMARK   3   VDW PROBE RADIUS   :   1.40
REMARK   3   ION PROBE RADIUS   :   0.80
REMARK   3   SHRINKAGE RADIUS   :   0.80
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: HYDROGENS HAVE BEEN ADDED IN THE
REMARK   3   RIDING POSITIONS
REMARK   4
REMARK   4 1H2K COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI  ON 12-AUG-2002.
REMARK 100 THE EBI ID CODE IS EBI-11170.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : 15-MAY-2002
REMARK 200  TEMPERATURE           (KELVIN) : 100
REMARK 200  PH                             : 7.5
REMARK 200  NUMBER OF CRYSTALS USED        : 1
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : Y
REMARK 200  RADIATION SOURCE               : SRS BEAMLINE PX9.6
REMARK 200  BEAMLINE                       : PX9.6
REMARK 200  X-RAY GENERATOR MODEL          : NULL
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M
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REMARK 200  WAVELENGTH OR RANGE        (A) : 0.87
REMARK 200  MONOCHROMATOR                  : NULL
REMARK 200  OPTICS                         : NULL
REMARK 200
REMARK 200  DETECTOR TYPE                  : CCD
REMARK 200  DETECTOR MANUFACTURER          : ADSC
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : MOSFLM
REMARK 200  DATA SCALING SOFTWARE          : SCALA
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 30574
REMARK 200  RESOLUTION RANGE HIGH      (A) : 2.15
REMARK 200  RESOLUTION RANGE LOW       (A) : 18.17
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : NONE
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : 99.2
REMARK 200  DATA REDUNDANCY                : 6.3
REMARK 200  R MERGE                    (I) : 0.052
REMARK 200  R SYM                      (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : 9.9
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.15
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.27
REMARK 200  COMPLETENESS FOR SHELL     (%) : 96.0
REMARK 200  DATA REDUNDANCY IN SHELL       : 3.4
REMARK 200  R MERGE FOR SHELL          (I) : 0.331
REMARK 200  R SYM FOR SHELL            (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR SHELL         : 1.5
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD
REMARK 200 SOFTWARE USED: SOLVE
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 63
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE, 4% PEG400,
REMARK 280  0.1M HEPES PH7.5, ARGON ATMOSPHERE, 11MG/ML PROTEIN WITH
REMARK 280  1MM FE(II), 2.5MM NOG AND 2.5MM PEPTIDE
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
REMARK 290       2555   -X,-Y,1/2+Z
REMARK 290       3555   1/2-Y,1/2+X,1/4+Z
REMARK 290       4555   1/2+Y,1/2-X,3/4+Z
REMARK 290       5555   1/2-X,1/2+Y,1/4-Z
REMARK 290       6555   1/2+X,1/2-Y,3/4-Z
REMARK 290       7555   Y,X,-Z
REMARK 290       8555   -Y,-X,1/2-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
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REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000       73.32800
REMARK 290   SMTRY1   3  0.000000 -1.000000  0.000000       43.08050
REMARK 290   SMTRY2   3  1.000000  0.000000  0.000000       43.08050
REMARK 290   SMTRY3   3  0.000000  0.000000  1.000000       36.66400
REMARK 290   SMTRY1   4  0.000000  1.000000  0.000000       43.08050
REMARK 290   SMTRY2   4 -1.000000  0.000000  0.000000       43.08050
REMARK 290   SMTRY3   4  0.000000  0.000000  1.000000      109.99200
REMARK 290   SMTRY1   5 -1.000000  0.000000  0.000000       43.08050
REMARK 290   SMTRY2   5  0.000000  1.000000  0.000000       43.08050
REMARK 290   SMTRY3   5  0.000000  0.000000 -1.000000       36.66400
REMARK 290   SMTRY1   6  1.000000  0.000000  0.000000       43.08050
REMARK 290   SMTRY2   6  0.000000 -1.000000  0.000000       43.08050
REMARK 290   SMTRY3   6  0.000000  0.000000 -1.000000      109.99200
REMARK 290   SMTRY1   7  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY2   7  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY3   7  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   8  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY2   8 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY3   8  0.000000  0.000000 -1.000000       73.32800
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF   2 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 300
REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC
REMARK 300
REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S
REMARK 300 PRODUCES A TETRAMER.
REMARK 300
REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE
REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT
REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE
REMARK 300 HOMODIMER OF CHAIN A
REMARK 300
REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS
REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH
REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
REMARK 300 THE CHAIN IN THE COMPLEX IS     2203.4 ANGSTROM**2
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
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REMARK 350 BIOMOLECULE:  1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 350   BIOMT1   2  0.000000 -1.000000  0.000000       86.16100
REMARK 350   BIOMT2   2 -1.000000  0.000000  0.000000       86.16100
REMARK 350   BIOMT3   2  0.000000  0.000000 -1.000000       73.32800
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465     MET A     1
REMARK 465     ALA A     2
REMARK 465     ALA A     3
REMARK 465     THR A     4
REMARK 465     ALA A     5
REMARK 465     ALA A     6
REMARK 465     GLU A     7
REMARK 465     ALA A     8
REMARK 465     VAL A     9
REMARK 465     ALA A    10
REMARK 465     SER A    11
REMARK 465     GLY A    12
REMARK 465     SER A    13
REMARK 465     GLY A    14
REMARK 465     LYS A   304
REMARK 465     ARG A   305
REMARK 465     ILE A   306
REMARK 465     SER S   786
REMARK 465     MET S   787
REMARK 465     ASP S   788
REMARK 465     GLU S   789
REMARK 465     SER S   790
REMARK 465     GLY S   791
REMARK 465     LEU S   792
REMARK 465     PRO S   793
REMARK 465     GLN S   794
REMARK 465     GLN S   807
REMARK 465     GLY S   808
REMARK 465     SER S   809
REMARK 465     ARG S   810
REMARK 465     ASN S   811
REMARK 465     GLN S   824
REMARK 465     VAL S   825
REMARK 465     ASN S   826
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470   M RES CSSEQI  ATOMS
REMARK 470     GLU A  15    CG   CD   OE1  OE2
REMARK 470     GLU A  29    CG   CD   OE1  OE2
REMARK 470     ASN A  87    CG   OD1  ND2
REMARK 470     LYS A 106    CD   CE   NZ
REMARK 470     LYS A 115    CG   CD   CE   NZ
REMARK 470     ARG A 117    CG   CD   NE   CZ   NH1  NH2
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REMARK 470     GLN A 133    CG   CD   OE1  NE2
REMARK 470     GLN A 136    CG   CD   OE1  NE2
REMARK 470     GLN A 137    CG   CD   OE1  NE2
REMARK 470     ARG A 156    CG   CD   NE   CZ   NH1  NH2
REMARK 470     LYS A 157    CD   CE   NZ
REMARK 470     LYS A 311    CG   CD   CE   NZ
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1   ATM2   ATM3
REMARK 500    ASN A  84   N    -  CA   -  C    ANGL. DEV. =    9.3 DEGREES
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 500 NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,1X,2(A4,A1,3X),12X,F5.3)
REMARK 500
REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1   RES CSSEQI ATM2   DEVIATION
REMARK 500    MET A 343  SD     MET A 343  CE      -0.249
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500  ATM1  RES C  SSEQI   ATM2  RES C  SSEQI          DISTANCE
REMARK 500
REMARK 500   O    GLN A   209     O    HOH Z   108              2.20
REMARK 525
REMARK 525 SOLVENT
REMARK 525
REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
REMARK 525 ASSOCIATED WITH:
REMARK 525   PROTEIN CHAIN  SOLVENT CHAIN
REMARK 525     A              Z
REMARK 525     S              H
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REMARK 525
REMARK 525 THE FOLLOWING SOLVENT MOLECULES LIE FARTHER THAN EXPECTED
REMARK 525 FROM THE PROTEIN OR NUCLEIC ACID MOLECULE AND MAY BE
REMARK 525 ASSOCIATED WITH A SYMMETRY RELATED MOLECULE (M=MODEL
REMARK 525 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 525 NUMBER; I=INSERTION CODE):
REMARK 525
REMARK 525 THESE MOLECULES CAN BE PLACED WITHIN  5.00 ANGSTROM OF THE
REMARK 525 OBSERVED OLIGOMER BY APPLYING THE SYMMETRY TRANSFORMATION
REMARK 525 INDICATED.
REMARK 525
REMARK 525  M RES CSSEQI     ORIGINAL COORDINATES    SYMMETRY TRANS.     DIST.
REMARK 525                     X       Y       Z
REMARK 525  1 HOH W 531    12.359  41.757  15.368     005       545       2.38
REMARK 525  1 HOH W 609    10.971  45.216  18.991     005       545       3.25
REMARK 525  1 HOH W 576    42.075  52.163  47.994     008       665       2.28
REMARK 525  1 HOH W 687    28.879   5.577  12.106     005       555       2.82
REMARK 525  1 HOH W 674    24.396  12.792   8.360     005       555       3.20
REMARK 525  1 HOH W 543    27.797   7.178  14.664     005       555       2.83
REMARK 525  1 HOH W 607    26.874  53.406  28.524     008       665       2.97
REMARK 600
REMARK 600 HETEROGEN
REMARK 600
REMARK 600 FOR METAL ATOM FE   FE2 A1350  THE COORDINATION ANGLES ARE:
REMARK 600  1 HIS   199A  NE2
REMARK 600  2 ASP   201A  OD2       104.0
REMARK 600  3 HIS   279A  NE2        85.8  88.0
REMARK 600  4 OGA  1351A  O2        163.5  92.4  96.8
REMARK 600  5 OGA  1351A  O2'        86.4 168.8  97.0  77.1
REMARK 600                           1     2     3     4
REMARK 700
REMARK 700 SHEET
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
REMARK 700 TWO SHEETS ARE DEFINED.
REMARK 800
REMARK 800 SITE
REMARK 800 SITE_IDENTIFIER: FE1
REMARK 800 SITE_DESCRIPTION: FE BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: OGA
REMARK 800 SITE_DESCRIPTION: OGA BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: SO1
REMARK 800 SITE_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: SO2
REMARK 800 SITE_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1D7G   RELATED DB: PDB
REMARK 900  A MODEL FOR THE COMPLEX BETWEEN THE
REMARK 900  HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS
REMARK 900   CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE
REMARK 900 RELATED ID: 1H2L   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2M   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2N   RELATED DB: PDB
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REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1L8C   RELATED DB: PDB
REMARK 900  STRUCTURAL BASIS FOR HIF-1ALPHA/CBP
REMARK 900  RECOGNITION IN THECELLULAR HYPOXIC RESPONSE
REMARK 900 RELATED ID: 1LM8   RELATED DB: PDB
REMARK 900  STRUCTURE OF A HIF-1A-PVHL-ELONGINB-
REMARK 900  ELONGINC COMPLEX
REMARK 900 RELATED ID: 1LQB   RELATED DB: PDB
REMARK 900  CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1
REMARK 900  ALPHA PEPTIDEBOUND TO THE PVHL/ELONGIN-C/
REMARK 900  ELONGIN-B COMPLEX
DBREF  1H2K A    1   349  SWS    Q969Q7   Q969Q7           1    349
DBREF  1H2K S  786   826  SWS    Q16665   HIFA_HUMAN     786    826
SEQRES   1 A  349  MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
SEQRES   2 A  349  GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEQRES   3 A  349  TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
SEQRES   4 A  349  ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
SEQRES   5 A  349  GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
SEQRES   6 A  349  ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
SEQRES   7 A  349  GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
SEQRES   8 A  349  VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
SEQRES   9 A  349  GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
SEQRES  10 A  349  SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
SEQRES  11 A  349  LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
SEQRES  12 A  349  LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
SEQRES  13 A  349  LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP
SEQRES  14 A  349  ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
SEQRES  15 A  349  THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEQRES  16 A  349  THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA
SEQRES  17 A  349  GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
SEQRES  18 A  349  ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
SEQRES  19 A  349  PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
SEQRES  20 A  349  ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY
SEQRES  21 A  349  TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE
SEQRES  22 A  349  PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN
SEQRES  23 A  349  GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY
SEQRES  24 A  349  ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA
SEQRES  25 A  349  HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET
SEQRES  26 A  349  LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
SEQRES  27 A  349  LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
SEQRES   1 S   41  SER MET ASP GLU SER GLY LEU PRO GLN LEU THR SER TYR
SEQRES   2 S   41  ASP CYS GLU VAL ASN ALA PRO ILE GLN GLY SER ARG ASN
SEQRES   3 S   41  LEU LEU GLN GLY GLU GLU LEU LEU ARG ALA LEU ASP GLN
SEQRES   4 S   41  VAL ASN
HET    FE2  A1350       1
HET    OGA  A1351      10
HET    SO4  A1352       5
HET    SO4  A1353       5
HETNAM     FE2 FE (II) ION
HETNAM     OGA N-OXALYOLGLYCINE
HETNAM     SO4 SULFATE ION
FORMUL   3  FE2     FE1 2+
FORMUL   4  OGA     C4 H5 N1 O5
FORMUL   5  SO4     2(O4 S1 2-)
FORMUL   6  HOH   *194(H2 O1)
HELIX    1   1 ASP A   28  LEU A   32  5                                   5
HELIX    2   2 ASP A   49  ASN A   58  1                                  10
HELIX    3   3 VAL A   70  TRP A   76  5                                   7
HELIX    4   4 ASP A   77  ILE A   85  1                                   9
HELIX    5   5 ASP A  104  GLN A  112  5                                   9
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HELIX    6   6 LYS A  124  ARG A  138  1                                          15
HELIX    7   7 GLY A  155  GLY A  164  1                                          10
HELIX    8   8 ASN A  166  GLY A  178  1                                          13
HELIX    9   9 PRO A  220  ASP A  222  5                                           3
HELIX   10  10 GLN A  223  TYR A  228  1                                           6
HELIX   11  11 PHE A  252  VAL A  258  5                                           7
HELIX   12  12 LYS A  311  GLY A  331  1                                          21
HELIX   13  13 ASN A  332  GLN A  334  5                                           3
HELIX   14  14 GLU A  335  LYS A  345  1                                          11
HELIX   15  15 GLN S  814  ASP S  823  1                                          10
SHEET    1  AA 5 THR A  39   PRO A  41   0
SHEET    2  AA 5 GLY A 260   VAL A 265   1  O  GLY A 260   N  ARG A  40
SHEET    3  AA 5 LYS A 214   PHE A 219  -1  O  LYS A 214   N  VAL A 265
SHEET    4  AA 5 TRP A 278   SER A 283  -1  O  TRP A 278   N  PHE A 219
SHEET    5  AA 5 VAL A 195   HIS A 199  -1  O  THR A 196   N  ILE A 281
SHEET    1  AB 6 ARG A  44   LEU A  45   0
SHEET    2  AB 6 VAL A  62   LEU A  64   1  O  VAL A  63   N  LEU A  45
SHEET    3  AB 6 VAL A 270   ILE A 273  -1  O  VAL A 270   N  LEU A  64
SHEET    4  AB 6 GLN A 203   LYS A 211  -1  O  ASN A 205   N  ILE A 273
SHEET    5  AB 6 THR A 290   LYS A 298  -1  O  ILE A 291   N  ILE A 210
SHEET    6  AB 6 LEU A 182   SER A 184  -1  N  THR A 183   O  TRP A 296
SHEET    1  AC 9 ARG A  44   LEU A  45   0
SHEET    2  AC 9 VAL A  62   LEU A  64   1  O  VAL A  63   N  LEU A  45
SHEET    3  AC 9 VAL A 270   ILE A 273  -1  O  VAL A 270   N  LEU A  64
SHEET    4  AC 9 GLN A 203   LYS A 211  -1  O  ASN A 205   N  ILE A 273
SHEET    5  AC 9 THR A 290   LYS A 298  -1  O  ILE A 291   N  ILE A 210
SHEET    6  AC 9 LEU A 186   GLY A 190  -1  O  LEU A 186   N  ASN A 294
SHEET    7  AC 9 ARG A 143   THR A 149  -1  O  LEU A 146   N  ILE A 189
SHEET    8  AC 9 PHE A  90   ALA A  95  -1  O  SER A  91   N  GLN A 147
SHEET    9  AC 9 SER A 118   MET A 123  -1  O  ASN A 119   N  SER A  94
LINK         FE   FE2 A1350                 NE2 HIS A 199     1555   1555  2.12
LINK         FE   FE2 A1350                 OD2 ASP A 201     1555   1555  2.05
LINK         FE   FE2 A1350                 NE2 HIS A 279     1555   1555  2.08
LINK         FE   FE2 A1350                 O2  OGA A1351     1555   1555  2.13
LINK         FE   FE2 A1350                 O2' OGA A1351     1555   1555  2.17
CISPEP   1 TYR A  308    PRO A  309          0        -1.09
SITE     1 FE1  3 HIS A 199  ASP A 201  HIS A 279
SITE     1 OGA 11 TYR A 145  THR A 196  HIS A 199  ASP A 201
SITE     2 OGA 11 ASN A 205  PHE A 207  LYS A 214  HIS A 279
SITE     3 OGA 11 ILE A 281  ASN A 294  TRP A 296
SITE     1 SO1  4 ARG A 138  GLY A 140  GLU A 141  GLU A 142
SITE     1 SO2  5 ARG A 143  GLU A 192  GLY A 193  LEU A 285
SITE     2 SO2  5 ASN A 286
CRYST1   86.161   86.161  146.656  90.00  90.00  90.00 P 41 21 2     8
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.011606  0.000000  0.000000        0.00000
SCALE2      0.000000  0.011606  0.000000        0.00000
SCALE3      0.000000  0.000000  0.006819        0.00000
ATOM      1  N   GLU A  15       8.429  32.653   9.844  1.00 50.99           N
ATOM      2  CA  GLU A  15       7.077  32.034   9.723  1.00 51.05           C
ATOM      3  C   GLU A  15       7.166  30.582  10.163  1.00 50.79           C
ATOM      4  O   GLU A  15       8.052  29.857   9.730  1.00 51.18           O
ATOM      5  CB  GLU A  15       6.570  32.124   8.296  1.00 51.20           C
ATOM      6  N   PRO A  16       6.254  30.150  11.022  1.00 50.50           N
ATOM      7  CA  PRO A  16       6.301  28.781  11.549  1.00 50.12           C
ATOM      8  C   PRO A  16       6.265  27.737  10.438  1.00 49.56           C
ATOM      9  O   PRO A  16       5.471  27.827   9.503  1.00 49.32           O
ATOM     10  CB  PRO A  16       5.049  28.701  12.429  1.00 50.27           C
ATOM     11  CG  PRO A  16       4.734  30.135  12.770  1.00 50.58           C
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ATOM     12  CD  PRO A  16       5.108  30.911  11.548  1.00 50.56           C
ATOM     13  N   ARG A  17       7.133  26.746  10.550  1.00 48.83           N
ATOM     14  CA  ARG A  17       7.219  25.695   9.550  1.00 48.33           C
ATOM     15  C   ARG A  17       5.967  24.832   9.561  1.00 47.48           C
ATOM     16  O   ARG A  17       5.245  24.782  10.557  1.00 47.64           O
ATOM     17  CB  ARG A  17       8.421  24.798   9.835  1.00 48.61           C
ATOM     18  CG  ARG A  17       9.776  25.511   9.835  1.00 49.21           C
ATOM     19  CD  ARG A  17      10.944  24.577  10.196  1.00 49.84           C
ATOM     20  NE  ARG A  17      10.918  24.137  11.596  1.00 50.12           N
ATOM     21  CZ  ARG A  17      11.455  24.809  12.623  1.00 50.99           C
ATOM     22  NH1 ARG A  17      12.065  25.979  12.431  1.00 50.40           N
ATOM     23  NH2 ARG A  17      11.381  24.310  13.857  1.00 50.81           N
ATOM     24  N   GLU A  18       5.723  24.153   8.446  1.00 46.05           N
ATOM     25  CA  GLU A  18       4.603  23.246   8.329  1.00 45.06           C
ATOM     26  C   GLU A  18       5.096  21.830   8.607  1.00 44.00           C
ATOM     27  O   GLU A  18       6.101  21.405   8.044  1.00 43.89           O
ATOM     28  CB  GLU A  18       4.013  23.324   6.923  1.00 45.21           C
ATOM     29  CG  GLU A  18       3.323  24.648   6.621  1.00 45.56           C
ATOM     30  CD  GLU A  18       1.951  24.780   7.265  1.00 45.64           C
ATOM     31  OE1 GLU A  18       1.342  23.749   7.641  1.00 44.14           O
ATOM     32  OE2 GLU A  18       1.480  25.932   7.388  1.00 45.83           O
ATOM     33  N   GLU A  19       4.396  21.113   9.484  1.00 42.49           N
ATOM     34  CA  GLU A  19       4.734  19.728   9.795  1.00 41.55           C
ATOM     35  C   GLU A  19       4.357  18.817   8.635  1.00 39.79           C
ATOM     36  O   GLU A  19       3.266  18.933   8.066  1.00 39.13           O
ATOM     37  CB  GLU A  19       4.010  19.256  11.052  1.00 41.88           C
ATOM     38  CG  GLU A  19       4.420  19.997  12.311  1.00 44.80           C
ATOM     39  CD  GLU A  19       4.276  19.155  13.574  1.00 49.28           C
ATOM     40  OE1 GLU A  19       3.759  18.008  13.497  1.00 51.52           O
ATOM     41  OE2 GLU A  19       4.695  19.643  14.656  1.00 52.76           O
ATOM     42  N   ALA A  20       5.270  17.910   8.311  1.00 38.00           N
ATOM     43  CA  ALA A  20       5.099  16.952   7.227  1.00 36.77           C
ATOM     44  C   ALA A  20       3.803  16.168   7.373  1.00 35.56           C
ATOM     45  O   ALA A  20       3.445  15.734   8.460  1.00 35.74           O
ATOM     46  CB  ALA A  20       6.283  15.999   7.180  1.00 36.63           C
ATOM     47  N   GLY A  21       3.082  16.020   6.279  1.00 34.05           N
ATOM     48  CA  GLY A  21       1.860  15.242   6.307  1.00 33.24           C
ATOM     49  C   GLY A  21       0.666  16.137   6.551  1.00 32.36           C
ATOM     50  O   GLY A  21      -0.393  15.673   6.951  1.00 30.93           O
ATOM     51  N   ALA A  22       0.867  17.432   6.323  1.00 32.41           N
ATOM     52  CA  ALA A  22      -0.184  18.425   6.459  1.00 32.78           C
ATOM     53  C   ALA A  22      -0.723  18.441   7.873  1.00 33.14           C
ATOM     54  O   ALA A  22      -1.915  18.605   8.088  1.00 32.74           O
ATOM     55  CB  ALA A  22      -1.304  18.139   5.462  1.00 32.61           C
ATOM     56  N   LEU A  23       0.151  18.253   8.849  1.00 34.01           N
ATOM     57  CA  LEU A  23      -0.297  18.275  10.232  1.00 34.91           C
ATOM     58  C   LEU A  23      -0.342  19.694  10.757  1.00 35.27           C
ATOM     59  O   LEU A  23      -0.528  19.918  11.943  1.00 35.72           O
ATOM     60  CB  LEU A  23       0.565  17.366  11.097  1.00 35.27           C
ATOM     61  CG  LEU A  23       0.384  15.910  10.653  1.00 36.36           C
ATOM     62  CD1 LEU A  23       1.211  14.947  11.491  1.00 37.75           C
ATOM     63  CD2 LEU A  23      -1.077  15.523  10.719  1.00 37.98           C
ATOM     64  N   GLY A  24      -0.177  20.656   9.855  1.00 35.73           N
ATOM     65  CA  GLY A  24      -0.332  22.053  10.194  1.00 35.66           C
ATOM     66  C   GLY A  24       0.901  22.655  10.804  1.00 36.08           C
ATOM     67  O   GLY A  24       1.945  22.001  10.913  1.00 36.05           O
ATOM     68  N   PRO A  25       0.764  23.894  11.253  1.00 35.96           N
ATOM     69  CA  PRO A  25       1.896  24.628  11.804  1.00 36.12           C
ATOM     70  C   PRO A  25       2.327  23.980  13.108  1.00 36.32           C
ATOM     71  O   PRO A  25       1.488  23.577  13.914  1.00 36.08           O
ATOM     72  CB  PRO A  25       1.341  26.047  12.043  1.00 36.15           C
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ATOM     73  CG  PRO A  25      -0.162  25.942  11.982  1.00 35.84           C
ATOM     74  CD  PRO A  25      -0.504  24.638  11.350  1.00 36.22           C
ATOM     75  N   ALA A  26       3.632  23.848  13.285  1.00 36.64           N
ATOM     76  CA  ALA A  26       4.178  23.274  14.499  1.00 37.19           C
ATOM     77  C   ALA A  26       3.860  24.172  15.706  1.00 36.77           C
ATOM     78  O   ALA A  26       3.595  23.678  16.808  1.00 37.19           O
ATOM     79  CB  ALA A  26       5.672  23.099  14.347  1.00 37.52           C
ATOM     80  N   TRP A  27       3.848  25.479  15.484  1.00 35.62           N
ATOM     81  CA  TRP A  27       3.520  26.420  16.543  1.00 35.04           C
ATOM     82  C   TRP A  27       3.029  27.729  15.933  1.00 34.20           C
ATOM     83  O   TRP A  27       2.992  27.883  14.723  1.00 33.57           O
ATOM     84  CB  TRP A  27       4.774  26.672  17.382  1.00 35.28           C
ATOM     85  CG  TRP A  27       5.951  26.889  16.511  1.00 34.67           C
ATOM     86  CD1 TRP A  27       6.761  25.930  15.955  1.00 35.52           C
ATOM     87  CD2 TRP A  27       6.426  28.135  16.033  1.00 34.40           C
ATOM     88  NE1 TRP A  27       7.723  26.522  15.172  1.00 35.09           N
ATOM     89  CE2 TRP A  27       7.541  27.877  15.209  1.00 34.23           C
ATOM     90  CE3 TRP A  27       6.038  29.452  16.232  1.00 34.31           C
ATOM     91  CZ2 TRP A  27       8.255  28.879  14.592  1.00 35.79           C
ATOM     92  CZ3 TRP A  27       6.750  30.442  15.629  1.00 36.35           C
ATOM     93  CH2 TRP A  27       7.847  30.154  14.808  1.00 36.47           C
ATOM     94  N   ASP A  28       2.638  28.672  16.766  1.00 33.77           N
ATOM     95  CA  ASP A  28       2.259  29.970  16.249  1.00 33.48           C
ATOM     96  C   ASP A  28       2.759  31.050  17.165  1.00 32.26           C
ATOM     97  O   ASP A  28       3.210  30.791  18.276  1.00 32.05           O
ATOM     98  CB  ASP A  28       0.749  30.080  16.037  1.00 34.30           C
ATOM     99  CG  ASP A  28      -0.026  29.986  17.317  1.00 36.29           C
ATOM    100  OD1 ASP A  28      -0.184  31.027  18.002  1.00 39.59           O
ATOM    101  OD2 ASP A  28      -0.517  28.906  17.712  1.00 39.78           O
ATOM    102  N   GLU A  29       2.691  32.268  16.654  1.00 31.30           N
ATOM    103  CA  GLU A  29       3.181  33.465  17.326  1.00 30.15           C
ATOM    104  C   GLU A  29       2.674  33.625  18.752  1.00 28.85           C
ATOM    105  O   GLU A  29       3.407  34.036  19.621  1.00 28.58           O
ATOM    106  CB  GLU A  29       2.791  34.682  16.503  1.00 30.32           C
ATOM    107  N   SER A  30       1.414  33.313  18.992  1.00 27.95           N
ATOM    108  CA  SER A  30       0.845  33.501  20.320  1.00 27.46           C
ATOM    109  C   SER A  30       1.537  32.671  21.389  1.00 26.93           C
ATOM    110  O   SER A  30       1.312  32.907  22.567  1.00 26.79           O
ATOM    111  CB  SER A  30      -0.651  33.168  20.322  1.00 27.23           C
ATOM    112  OG  SER A  30      -0.857  31.764  20.306  1.00 27.69           O
ATOM    113  N   GLN A  31       2.360  31.703  20.984  1.00 26.55           N
ATOM    114  CA  GLN A  31       3.071  30.837  21.926  1.00 26.63           C
ATOM    115  C   GLN A  31       4.419  31.409  22.334  1.00 26.66           C
ATOM    116  O   GLN A  31       5.078  30.855  23.205  1.00 26.45           O
ATOM    117  CB  GLN A  31       3.282  29.426  21.349  1.00 26.41           C
ATOM    118  CG  GLN A  31       1.998  28.637  21.131  1.00 26.28           C
ATOM    119  CD  GLN A  31       2.245  27.287  20.489  1.00 26.25           C
ATOM    120  OE1 GLN A  31       2.258  27.183  19.271  1.00 27.92           O
ATOM    121  NE2 GLN A  31       2.465  26.258  21.305  1.00 24.36           N
ATOM    122  N   LEU A  32       4.824  32.508  21.703  1.00 26.89           N
ATOM    123  CA  LEU A  32       6.083  33.176  22.029  1.00 27.24           C
ATOM    124  C   LEU A  32       5.852  34.321  23.006  1.00 26.92           C
ATOM    125  O   LEU A  32       4.888  35.047  22.868  1.00 26.42           O
ATOM    126  CB  LEU A  32       6.717  33.746  20.760  1.00 27.46           C
ATOM    127  CG  LEU A  32       6.964  32.728  19.640  1.00 28.65           C
ATOM    128  CD1 LEU A  32       7.630  33.391  18.452  1.00 29.44           C
ATOM    129  CD2 LEU A  32       7.792  31.573  20.127  1.00 27.98           C
ATOM    130  N   ARG A  33       6.728  34.472  23.995  1.00 26.71           N
ATOM    131  CA  ARG A  33       6.627  35.596  24.923  1.00 26.77           C
ATOM    132  C   ARG A  33       7.040  36.880  24.209  1.00 26.57           C
ATOM    133  O   ARG A  33       7.719  36.844  23.203  1.00 26.30           O
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ATOM    134  CB  ARG A  33       7.492  35.357  26.163  1.00 26.67           C
ATOM    135  CG  ARG A  33       7.052  34.141  26.983  1.00 26.29           C
ATOM    136  CD  ARG A  33       7.937  33.837  28.181  1.00 25.85           C
ATOM    137  NE  ARG A  33       7.381  32.778  29.018  1.00 25.80           N
ATOM    138  CZ  ARG A  33       6.451  32.946  29.945  1.00 24.68           C
ATOM    139  NH1 ARG A  33       5.937  34.140  30.189  1.00 23.50           N
ATOM    140  NH2 ARG A  33       6.029  31.901  30.637  1.00 25.35           N
ATOM    141  N   SER A  34       6.633  38.020  24.732  1.00 26.80           N
ATOM    142  CA  SER A  34       6.903  39.280  24.061  1.00 27.15           C
ATOM    143  C   SER A  34       7.990  40.048  24.791  1.00 26.39           C
ATOM    144  O   SER A  34       7.964  40.140  26.005  1.00 25.87           O
ATOM    145  CB  SER A  34       5.628  40.104  24.030  1.00 27.68           C
ATOM    146  OG  SER A  34       5.494  40.737  25.285  1.00 32.47           O
ATOM    147  N   TYR A  35       8.944  40.589  24.042  1.00 25.89           N
ATOM    148  CA  TYR A  35      10.110  41.223  24.637  1.00 26.28           C
ATOM    149  C   TYR A  35      10.353  42.558  23.970  1.00 26.85           C
ATOM    150  O   TYR A  35       9.722  42.856  22.967  1.00 26.92           O
ATOM    151  CB  TYR A  35      11.326  40.308  24.510  1.00 25.90           C
ATOM    152  CG  TYR A  35      11.169  39.032  25.309  1.00 25.33           C
ATOM    153  CD1 TYR A  35      10.975  39.073  26.685  1.00 24.99           C
ATOM    154  CD2 TYR A  35      11.198  37.787  24.692  1.00 23.82           C
ATOM    155  CE1 TYR A  35      10.823  37.898  27.429  1.00 24.56           C
ATOM    156  CE2 TYR A  35      11.046  36.620  25.426  1.00 24.42           C
ATOM    157  CZ  TYR A  35      10.862  36.682  26.793  1.00 23.48           C
ATOM    158  OH  TYR A  35      10.696  35.524  27.513  1.00 24.75           O
ATOM    159  N   SER A  36      11.304  43.327  24.496  1.00 27.27           N
ATOM    160  CA  SER A  36      11.525  44.704  24.052  1.00 27.55           C
ATOM    161  C   SER A  36      12.513  44.912  22.917  1.00 27.06           C
ATOM    162  O   SER A  36      12.734  46.049  22.504  1.00 27.94           O
ATOM    163  CB  SER A  36      12.082  45.498  25.226  1.00 27.88           C
ATOM    164  OG  SER A  36      13.350  44.976  25.590  1.00 28.36           O
ATOM    165  N   PHE A  37      13.128  43.851  22.429  1.00 25.35           N
ATOM    166  CA  PHE A  37      14.202  44.014  21.461  1.00 24.62           C
ATOM    167  C   PHE A  37      13.899  43.272  20.159  1.00 24.75           C
ATOM    168  O   PHE A  37      13.130  42.335  20.135  1.00 24.25           O
ATOM    169  CB  PHE A  37      15.487  43.462  22.071  1.00 23.87           C
ATOM    170  CG  PHE A  37      15.318  42.069  22.635  1.00 22.53           C
ATOM    171  CD1 PHE A  37      15.348  40.972  21.802  1.00 21.11           C
ATOM    172  CD2 PHE A  37      15.069  41.872  23.988  1.00 21.63           C
ATOM    173  CE1 PHE A  37      15.158  39.687  22.314  1.00 22.41           C
ATOM    174  CE2 PHE A  37      14.900  40.612  24.505  1.00 22.29           C
ATOM    175  CZ  PHE A  37      14.936  39.509  23.675  1.00 21.45           C
ATOM    176  N   PRO A  38      14.489  43.715  19.067  1.00 24.94           N
ATOM    177  CA  PRO A  38      14.322  43.017  17.793  1.00 24.67           C
ATOM    178  C   PRO A  38      15.267  41.823  17.678  1.00 24.41           C
ATOM    179  O   PRO A  38      16.249  41.745  18.427  1.00 23.73           O
ATOM    180  CB  PRO A  38      14.725  44.072  16.783  1.00 24.75           C
ATOM    181  CG  PRO A  38      15.791  44.872  17.530  1.00 26.09           C
ATOM    182  CD  PRO A  38      15.287  44.950  18.941  1.00 25.27           C
ATOM    183  N   THR A  39      14.981  40.927  16.734  1.00 23.30           N
ATOM    184  CA  THR A  39      15.859  39.816  16.444  1.00 23.42           C
ATOM    185  C   THR A  39      15.857  39.534  14.955  1.00 24.29           C
ATOM    186  O   THR A  39      14.958  39.964  14.239  1.00 24.61           O
ATOM    187  CB  THR A  39      15.368  38.538  17.135  1.00 23.09           C
ATOM    188  OG1 THR A  39      14.044  38.232  16.680  1.00 19.92           O
ATOM    189  CG2 THR A  39      15.213  38.731  18.641  1.00 23.03           C
ATOM    190  N   ARG A  40      16.854  38.773  14.525  1.00 24.43           N
ATOM    191  CA  ARG A  40      16.982  38.273  13.170  1.00 24.91           C
ATOM    192  C   ARG A  40      17.061  36.751  13.268  1.00 24.49           C
ATOM    193  O   ARG A  40      17.434  36.225  14.301  1.00 23.58           O
ATOM    194  CB  ARG A  40      18.253  38.805  12.536  1.00 25.36           C
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ATOM    195  CG  ARG A  40      18.208  40.281  12.248  1.00 30.74           C
ATOM    196  CD  ARG A  40      16.823  40.775  11.890  1.00 34.86           C
ATOM    197  NE  ARG A  40      16.604  40.989  10.477  1.00 39.38           N
ATOM    198  CZ  ARG A  40      15.403  41.229   9.971  1.00 43.86           C
ATOM    199  NH1 ARG A  40      14.345  41.254  10.782  1.00 45.88           N
ATOM    200  NH2 ARG A  40      15.252  41.457   8.674  1.00 44.96           N
ATOM    201  N   PRO A  41      16.687  36.031  12.221  1.00 25.08           N
ATOM    202  CA  PRO A  41      16.715  34.565  12.290  1.00 25.39           C
ATOM    203  C   PRO A  41      18.095  33.913  12.282  1.00 25.10           C
ATOM    204  O   PRO A  41      19.007  34.370  11.636  1.00 25.16           O
ATOM    205  CB  PRO A  41      15.953  34.130  11.023  1.00 25.76           C
ATOM    206  CG  PRO A  41      15.286  35.392  10.504  1.00 26.54           C
ATOM    207  CD  PRO A  41      16.151  36.524  10.939  1.00 24.85           C
ATOM    208  N   ILE A  42      18.225  32.823  13.020  1.00 25.28           N
ATOM    209  CA  ILE A  42      19.388  31.974  12.919  1.00 24.31           C
ATOM    210  C   ILE A  42      19.147  31.116  11.677  1.00 24.68           C
ATOM    211  O   ILE A  42      18.043  30.614  11.466  1.00 24.72           O
ATOM    212  CB  ILE A  42      19.481  31.104  14.163  1.00 24.80           C
ATOM    213  CG1 ILE A  42      19.763  31.993  15.384  1.00 24.24           C
ATOM    214  CG2 ILE A  42      20.530  30.004  13.961  1.00 23.81           C
ATOM    215  CD1 ILE A  42      19.531  31.325  16.729  1.00 23.59           C
ATOM    216  N   PRO A  43      20.146  30.953  10.826  1.00 24.48           N
ATOM    217  CA  PRO A  43      19.963  30.108   9.651  1.00 24.60           C
ATOM    218  C   PRO A  43      19.611  28.650  10.001  1.00 24.85           C
ATOM    219  O   PRO A  43      20.148  28.130  10.989  1.00 24.38           O
ATOM    220  CB  PRO A  43      21.320  30.192   8.937  1.00 24.87           C
ATOM    221  CG  PRO A  43      22.040  31.372   9.541  1.00 25.04           C
ATOM    222  CD  PRO A  43      21.475  31.583  10.886  1.00 24.37           C
ATOM    223  N   ARG A  44      18.686  28.032   9.248  1.00 24.70           N
ATOM    224  CA  ARG A  44      18.367  26.608   9.391  1.00 25.53           C
ATOM    225  C   ARG A  44      18.910  25.943   8.152  1.00 25.00           C
ATOM    226  O   ARG A  44      18.505  26.265   7.030  1.00 24.62           O
ATOM    227  CB  ARG A  44      16.873  26.287   9.452  1.00 26.51           C
ATOM    228  CG  ARG A  44      16.044  27.133  10.378  1.00 29.49           C
ATOM    229  CD  ARG A  44      14.683  26.485  10.813  1.00 31.03           C
ATOM    230  NE  ARG A  44      14.401  25.120  10.323  1.00 32.36           N
ATOM    231  CZ  ARG A  44      14.174  24.057  11.126  1.00 33.85           C
ATOM    232  NH1 ARG A  44      14.239  24.170  12.451  1.00 30.71           N
ATOM    233  NH2 ARG A  44      13.898  22.863  10.613  1.00 35.56           N
ATOM    234  N   LEU A  45      19.815  25.006   8.337  1.00 23.91           N
ATOM    235  CA  LEU A  45      20.500  24.444   7.202  1.00 23.40           C
ATOM    236  C   LEU A  45      20.684  22.967   7.352  1.00 23.52           C
ATOM    237  O   LEU A  45      20.559  22.423   8.446  1.00 22.50           O
ATOM    238  CB  LEU A  45      21.888  25.064   7.093  1.00 22.62           C
ATOM    239  CG  LEU A  45      21.911  26.563   6.819  1.00 23.96           C
ATOM    240  CD1 LEU A  45      23.317  27.111   6.947  1.00 24.52           C
ATOM    241  CD2 LEU A  45      21.366  26.845   5.423  1.00 24.63           C
ATOM    242  N   SER A  46      21.018  22.347   6.227  1.00 23.57           N
ATOM    243  CA  SER A  46      21.382  20.975   6.221  1.00 24.12           C
ATOM    244  C   SER A  46      22.820  20.888   6.668  1.00 24.81           C
ATOM    245  O   SER A  46      23.640  21.757   6.398  1.00 23.76           O
ATOM    246  CB  SER A  46      21.236  20.354   4.830  1.00 23.80           C
ATOM    247  OG  SER A  46      21.744  19.020   4.830  1.00 24.09           O
ATOM    248  N   GLN A  47      23.089  19.804   7.366  1.00 25.92           N
ATOM    249  CA  GLN A  47      24.399  19.444   7.844  1.00 27.25           C
ATOM    250  C   GLN A  47      25.379  19.326   6.674  1.00 27.54           C
ATOM    251  O   GLN A  47      26.563  19.564   6.836  1.00 27.97           O
ATOM    252  CB  GLN A  47      24.245  18.088   8.554  1.00 28.46           C
ATOM    253  CG  GLN A  47      25.487  17.279   8.705  1.00 31.10           C
ATOM    254  CD  GLN A  47      25.776  16.372   7.570  1.00 33.17           C
ATOM    255  OE1 GLN A  47      24.881  15.970   6.803  1.00 36.23           O
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ATOM    256  NE2 GLN A  47      27.041  16.000   7.458  1.00 36.17           N
ATOM    257  N   SER A  48      24.884  18.951   5.498  1.00 27.72           N
ATOM    258  CA  SER A  48      25.736  18.809   4.323  1.00 28.35           C
ATOM    259  C   SER A  48      26.016  20.150   3.629  1.00 28.86           C
ATOM    260  O   SER A  48      26.825  20.235   2.711  1.00 28.96           O
ATOM    261  CB  SER A  48      25.092  17.839   3.324  1.00 28.65           C
ATOM    262  OG  SER A  48      23.798  18.276   2.918  1.00 28.51           O
ATOM    263  N   ASP A  49      25.347  21.203   4.065  1.00 29.16           N
ATOM    264  CA  ASP A  49      25.515  22.496   3.442  1.00 29.28           C
ATOM    265  C   ASP A  49      26.800  23.163   3.913  1.00 29.71           C
ATOM    266  O   ASP A  49      26.981  23.398   5.101  1.00 29.02           O
ATOM    267  CB  ASP A  49      24.325  23.369   3.783  1.00 29.35           C
ATOM    268  CG  ASP A  49      24.316  24.667   3.010  1.00 29.93           C
ATOM    269  OD1 ASP A  49      25.398  25.183   2.666  1.00 28.14           O
ATOM    270  OD2 ASP A  49      23.259  25.247   2.731  1.00 30.49           O
ATOM    271  N   PRO A  50      27.693  23.483   2.976  1.00 30.34           N
ATOM    272  CA  PRO A  50      28.964  24.134   3.315  1.00 30.54           C
ATOM    273  C   PRO A  50      28.783  25.354   4.186  1.00 30.38           C
ATOM    274  O   PRO A  50      29.661  25.651   4.990  1.00 30.53           O
ATOM    275  CB  PRO A  50      29.520  24.573   1.952  1.00 30.39           C
ATOM    276  CG  PRO A  50      28.926  23.667   0.988  1.00 30.96           C
ATOM    277  CD  PRO A  50      27.574  23.243   1.531  1.00 30.51           C
ATOM    278  N   ARG A  51      27.683  26.072   4.008  1.00 30.50           N
ATOM    279  CA  ARG A  51      27.439  27.253   4.817  1.00 30.94           C
ATOM    280  C   ARG A  51      27.341  26.875   6.299  1.00 30.49           C
ATOM    281  O   ARG A  51      27.744  27.646   7.161  1.00 29.74           O
ATOM    282  CB  ARG A  51      26.171  27.979   4.370  1.00 30.97           C
ATOM    283  CG  ARG A  51      26.337  28.781   3.099  1.00 33.47           C
ATOM    284  CD  ARG A  51      25.029  29.321   2.521  1.00 34.80           C
ATOM    285  NE  ARG A  51      24.071  28.252   2.221  1.00 36.68           N
ATOM    286  CZ  ARG A  51      22.766  28.448   2.081  1.00 37.94           C
ATOM    287  NH1 ARG A  51      22.260  29.677   2.208  1.00 39.10           N
ATOM    288  NH2 ARG A  51      21.967  27.436   1.794  1.00 36.51           N
ATOM    289  N   ALA A  52      26.831  25.684   6.596  1.00 30.03           N
ATOM    290  CA  ALA A  52      26.697  25.288   7.993  1.00 29.96           C
ATOM    291  C   ALA A  52      28.079  25.101   8.593  1.00 30.07           C
ATOM    292  O   ALA A  52      28.345  25.518   9.710  1.00 29.00           O
ATOM    293  CB  ALA A  52      25.901  24.028   8.119  1.00 29.81           C
ATOM    294  N   GLU A  53      28.958  24.455   7.845  1.00 30.12           N
ATOM    295  CA  GLU A  53      30.290  24.213   8.347  1.00 31.08           C
ATOM    296  C   GLU A  53      30.999  25.550   8.579  1.00 30.37           C
ATOM    297  O   GLU A  53      31.683  25.730   9.580  1.00 29.89           O
ATOM    298  CB  GLU A  53      31.086  23.362   7.379  1.00 31.41           C
ATOM    299  CG  GLU A  53      32.189  22.603   8.081  1.00 35.02           C
ATOM    300  CD  GLU A  53      31.785  21.185   8.507  1.00 37.87           C
ATOM    301  OE1 GLU A  53      30.614  20.929   8.887  1.00 39.16           O
ATOM    302  OE2 GLU A  53      32.674  20.313   8.463  1.00 40.43           O
ATOM    303  N   GLU A  54      30.811  26.479   7.652  1.00 29.84           N
ATOM    304  CA  GLU A  54      31.413  27.796   7.757  1.00 30.22           C
ATOM    305  C   GLU A  54      30.975  28.486   9.045  1.00 29.05           C
ATOM    306  O   GLU A  54      31.780  29.102   9.719  1.00 28.03           O
ATOM    307  CB  GLU A  54      31.026  28.680   6.573  1.00 30.53           C
ATOM    308  CG  GLU A  54      31.635  28.276   5.243  1.00 34.66           C
ATOM    309  CD  GLU A  54      30.993  29.002   4.058  1.00 38.49           C
ATOM    310  OE1 GLU A  54      30.651  30.208   4.214  1.00 42.20           O
ATOM    311  OE2 GLU A  54      30.829  28.368   2.975  1.00 41.54           O
ATOM    312  N   LEU A  55      29.696  28.366   9.387  1.00 28.24           N
ATOM    313  CA  LEU A  55      29.177  29.029  10.571  1.00 27.28           C
ATOM    314  C   LEU A  55      29.774  28.448  11.827  1.00 26.43           C
ATOM    315  O   LEU A  55      30.212  29.199  12.695  1.00 25.20           O
ATOM    316  CB  LEU A  55      27.655  28.975  10.597  1.00 27.25           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 317 | CG | LEU | A | 55 | 27.027 | 29.829 | 9.502 | 1.00 | 27.43 | C |
| ATOM | 318 | CD1 | LEU | A | 55 | 25.568 | 29.452 | 9.322 | 1.00 | 28.83 | C |
| ATOM | 319 | CD2 | LEU | A | 55 | 27.173 | 31.318 | 9.821 | 1.00 | 26.98 | C |
| ATOM | 320 | N | ILE | A | 56 | 29.829 | 27.116 | 11.915 | 1.00 | 25.75 | N |
| ATOM | 321 | CA | ILE | A | 56 | 30.382 | 26.473 | 13.107 | 1.00 | 25.50 | C |
| ATOM | 322 | C | ILE | A | 56 | 31.874 | 26.815 | 13.254 | 1.00 | 26.26 | C |
| ATOM | 323 | O | ILE | A | 56 | 32.346 | 27.134 | 14.349 | 1.00 | 25.55 | O |
| ATOM | 324 | CB | ILE | A | 56 | 30.192 | 24.955 | 13.059 | 1.00 | 25.63 | C |
| ATOM | 325 | CG1 | ILE | A | 56 | 28.698 | 24.574 | 13.034 | 1.00 | 24.00 | C |
| ATOM | 326 | CG2 | ILE | A | 56 | 30.848 | 24.321 | 14.263 | 1.00 | 25.48 | C |
| ATOM | 327 | CD1 | ILE | A | 56 | 28.439 | 23.170 | 12.531 | 1.00 | 24.10 | C |
| ATOM | 328 | N | GLU | A | 57 | 32.597 | 26.781 | 12.135 | 1.00 | 27.04 | N |
| ATOM | 329 | CA | GLU | A | 57 | 34.023 | 27.082 | 12.107 | 1.00 | 28.01 | C |
| ATOM | 330 | C | GLU | A | 57 | 34.232 | 28.491 | 12.625 | 1.00 | 28.49 | C |
| ATOM | 331 | O | GLU | A | 57 | 35.183 | 28.770 | 13.344 | 1.00 | 28.92 | O |
| ATOM | 332 | CB | GLU | A | 57 | 34.561 | 26.977 | 10.676 | 1.00 | 28.61 | C |
| ATOM | 333 | CG | GLU | A | 57 | 36.053 | 27.224 | 10.509 | 1.00 | 30.77 | C |
| ATOM | 334 | CD | GLU | A | 57 | 36.902 | 26.322 | 11.394 | 1.00 | 35.15 | C |
| ATOM | 335 | OE1 | GLU | A | 57 | 36.556 | 25.127 | 11.591 | 1.00 | 37.11 | O |
| ATOM | 336 | OE2 | GLU | A | 57 | 37.924 | 26.818 | 11.909 | 1.00 | 40.88 | O |
| ATOM | 337 | N | ASN | A | 58 | 33.321 | 29.378 | 12.270 | 1.00 | 28.34 | N |
| ATOM | 338 | CA | ASN | A | 58 | 33.424 | 30.758 | 12.701 | 1.00 | 28.81 | C |
| ATOM | 339 | C | ASN | A | 58 | 32.770 | 31.079 | 14.025 | 1.00 | 27.23 | C |
| ATOM | 340 | O | ASN | A | 58 | 32.630 | 32.233 | 14.374 | 1.00 | 26.07 | O |
| ATOM | 341 | CB | ASN | A | 58 | 32.792 | 31.641 | 11.656 | 1.00 | 29.66 | C |
| ATOM | 342 | CG | ASN | A | 58 | 33.789 | 32.386 | 10.913 | 1.00 | 33.61 | C |
| ATOM | 343 | OD1 | ASN | A | 58 | 34.280 | 31.901 | 9.893 | 1.00 | 38.81 | O |
| ATOM | 344 | ND2 | ASN | A | 58 | 34.160 | 33.582 | 11.429 | 1.00 | 36.72 | N |
| ATOM | 345 | N | GLU | A | 59 | 32.343 | 30.053 | 14.735 | 1.00 | 26.39 | N |
| ATOM | 346 | CA | GLU | A | 59 | 31.712 | 30.241 | 16.030 | 1.00 | 26.36 | C |
| ATOM | 347 | C | GLU | A | 59 | 30.495 | 31.144 | 15.926 | 1.00 | 25.39 | C |
| ATOM | 348 | O | GLU | A | 59 | 30.325 | 32.100 | 16.668 | 1.00 | 24.14 | O |
| ATOM | 349 | CB | GLU | A | 59 | 32.753 | 30.697 | 17.059 | 1.00 | 26.80 | C |
| ATOM | 350 | CG | GLU | A | 59 | 33.717 | 29.537 | 17.316 | 1.00 | 29.10 | C |
| ATOM | 351 | CD | GLU | A | 59 | 34.722 | 29.791 | 18.407 | 1.00 | 32.85 | C |
| ATOM | 352 | OE1 | GLU | A | 59 | 35.790 | 30.330 | 18.080 | 1.00 | 37.47 | O |
| ATOM | 353 | OE2 | GLU | A | 59 | 34.466 | 29.432 | 19.572 | 1.00 | 34.14 | O |
| ATOM | 354 | N | GLU | A | 60 | 29.641 | 30.799 | 14.970 | 1.00 | 24.88 | N |
| ATOM | 355 | CA | GLU | A | 60 | 28.366 | 31.465 | 14.801 | 1.00 | 25.20 | C |
| ATOM | 356 | C | GLU | A | 60 | 27.262 | 30.414 | 14.822 | 1.00 | 24.07 | C |
| ATOM | 357 | O | GLU | A | 60 | 27.420 | 29.320 | 14.293 | 1.00 | 22.49 | O |
| ATOM | 358 | CB | GLU | A | 60 | 28.343 | 32.249 | 13.505 | 1.00 | 25.69 | C |
| ATOM | 359 | CG | GLU | A | 60 | 29.354 | 33.363 | 13.536 | 1.00 | 30.40 | C |
| ATOM | 360 | CD | GLU | A | 60 | 28.962 | 34.516 | 12.657 | 1.00 | 37.91 | C |
| ATOM | 361 | OE1 | GLU | A | 60 | 29.009 | 34.377 | 11.414 | 1.00 | 38.24 | O |
| ATOM | 362 | OE2 | GLU | A | 60 | 28.595 | 35.566 | 13.236 | 1.00 | 46.50 | O |
| ATOM | 363 | N | PRO | A | 61 | 26.124 | 30.779 | 15.386 | 1.00 | 22.90 | N |
| ATOM | 364 | CA | PRO | A | 61 | 25.045 | 29.816 | 15.571 | 1.00 | 22.19 | C |
| ATOM | 365 | C | PRO | A | 61 | 24.448 | 29.371 | 14.267 | 1.00 | 21.47 | C |
| ATOM | 366 | O | PRO | A | 61 | 24.419 | 30.104 | 13.266 | 1.00 | 20.48 | O |
| ATOM | 367 | CB | PRO | A | 61 | 23.996 | 30.583 | 16.368 | 1.00 | 22.29 | C |
| ATOM | 368 | CG | PRO | A | 61 | 24.315 | 32.053 | 16.148 | 1.00 | 22.67 | C |
| ATOM | 369 | CD | PRO | A | 61 | 25.764 | 32.140 | 15.798 | 1.00 | 22.92 | C |
| ATOM | 370 | N | VAL | A | 62 | 23.957 | 28.142 | 14.283 | 1.00 | 20.87 | N |
| ATOM | 371 | CA | VAL | A | 62 | 23.248 | 27.591 | 13.146 | 1.00 | 20.94 | C |
| ATOM | 372 | C | VAL | A | 62 | 22.353 | 26.475 | 13.655 | 1.00 | 21.15 | C |
| ATOM | 373 | O | VAL | A | 62 | 22.714 | 25.761 | 14.605 | 1.00 | 21.21 | O |
| ATOM | 374 | CB | VAL | A | 62 | 24.214 | 27.052 | 12.073 | 1.00 | 21.30 | C |
| ATOM | 375 | CG1 | VAL | A | 62 | 25.061 | 25.912 | 12.608 | 1.00 | 22.10 | C |
| ATOM | 376 | CG2 | VAL | A | 62 | 23.440 | 26.587 | 10.825 | 1.00 | 21.19 | C |
| ATOM | 377 | N | VAL | A | 63 | 21.158 | 26.366 | 13.084 | 1.00 | 21.48 | N |

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ATOM    378  CA  VAL A  63      20.302  25.231  13.374  1.00 21.87           C
ATOM    379  C   VAL A  63      20.526  24.212  12.270  1.00 22.00           C
ATOM    380  O   VAL A  63      20.366  24.528  11.109  1.00 22.54           O
ATOM    381  CB  VAL A  63      18.793  25.574  13.421  1.00 22.02           C
ATOM    382  CG1 VAL A  63      17.955  24.277  13.612  1.00 21.90           C
ATOM    383  CG2 VAL A  63      18.494  26.522  14.546  1.00 21.22           C
ATOM    384  N   LEU A  64      20.911  23.002  12.643  1.00 22.48           N
ATOM    385  CA  LEU A  64      21.067  21.902  11.710  1.00 23.08           C
ATOM    386  C   LEU A  64      19.826  21.014  11.775  1.00 22.19           C
ATOM    387  O   LEU A  64      19.423  20.558  12.843  1.00 21.85           O
ATOM    388  CB  LEU A  64      22.327  21.107  12.032  1.00 24.00           C
ATOM    389  CG  LEU A  64      23.614  21.930  11.984  1.00 27.02           C
ATOM    390  CD1 LEU A  64      24.791  21.080  12.303  1.00 31.61           C
ATOM    391  CD2 LEU A  64      23.827  22.540  10.640  1.00 29.86           C
ATOM    392  N   THR A  65      19.222  20.757  10.628  1.00 21.50           N
ATOM    393  CA  THR A  65      17.943  20.056  10.613  1.00 21.95           C
ATOM    394  C   THR A  65      18.022  18.561  10.389  1.00 21.35           C
ATOM    395  O   THR A  65      17.028  17.870  10.581  1.00 21.37           O
ATOM    396  CB  THR A  65      17.062  20.592   9.478  1.00 22.08           C
ATOM    397  OG1 THR A  65      17.725  20.351   8.230  1.00 22.38           O
ATOM    398  CG2 THR A  65      16.919  22.099   9.553  1.00 24.00           C
ATOM    399  N   ASP A  66      19.168  18.062   9.961  1.00 21.50           N
ATOM    400  CA  ASP A  66      19.259  16.650   9.604  1.00 21.86           C
ATOM    401  C   ASP A  66      20.513  15.899  10.069  1.00 21.61           C
ATOM    402  O   ASP A  66      21.070  15.088   9.316  1.00 21.82           O
ATOM    403  CB  ASP A  66      19.152  16.553   8.084  1.00 22.20           C
ATOM    404  CG  ASP A  66      20.199  17.355   7.390  1.00 21.49           C
ATOM    405  OD1 ASP A  66      21.065  17.936   8.070  1.00 21.14           O
ATOM    406  OD2 ASP A  66      20.240  17.477   6.159  1.00 25.40           O
ATOM    407  N   THR A  67      20.967  16.158  11.287  1.00 21.05           N
ATOM    408  CA  THR A  67      22.154  15.491  11.768  1.00 20.85           C
ATOM    409  C   THR A  67      21.858  14.084  12.231  1.00 20.12           C
ATOM    410  O   THR A  67      22.757  13.281  12.283  1.00 20.45           O
ATOM    411  CB  THR A  67      22.747  16.207  12.977  1.00 20.77           C
ATOM    412  OG1 THR A  67      21.782  16.210  14.039  1.00 20.61           O
ATOM    413  CG2 THR A  67      23.054  17.671  12.682  1.00 22.44           C
ATOM    414  N   ASN A  68      20.614  13.815  12.618  1.00 19.51           N
ATOM    415  CA  ASN A  68      20.269  12.555  13.267  1.00 19.09           C
ATOM    416  C   ASN A  68      21.116  12.349  14.517  1.00 18.40           C
ATOM    417  O   ASN A  68      21.383  11.212  14.928  1.00 17.67           O
ATOM    418  CB  ASN A  68      20.455  11.362  12.325  1.00 19.63           C
ATOM    419  CG  ASN A  68      19.453  11.344  11.209  1.00 19.93           C
ATOM    420  OD1 ASN A  68      18.253  11.236  11.442  1.00 19.76           O
ATOM    421  ND2 ASN A  68      19.941  11.423   9.987  1.00 19.96           N
ATOM    422  N   LEU A  69      21.532  13.448  15.134  1.00 18.28           N
ATOM    423  CA  LEU A  69      22.378  13.382  16.326  1.00 17.98           C
ATOM    424  C   LEU A  69      21.773  12.542  17.447  1.00 17.59           C
ATOM    425  O   LEU A  69      22.478  11.725  18.039  1.00 17.61           O
ATOM    426  CB  LEU A  69      22.693  14.772  16.844  1.00 18.38           C
ATOM    427  CG  LEU A  69      23.636  14.859  18.035  1.00 18.31           C
ATOM    428  CD1 LEU A  69      24.936  14.144  17.744  1.00 20.68           C
ATOM    429  CD2 LEU A  69      23.907  16.299  18.399  1.00 19.25           C
ATOM    430  N   VAL A  70      20.489  12.741  17.740  1.00 17.27           N
ATOM    431  CA  VAL A  70      19.811  11.989  18.794  1.00 17.72           C
ATOM    432  C   VAL A  70      18.588  11.253  18.257  1.00 18.11           C
ATOM    433  O   VAL A  70      17.557  11.148  18.927  1.00 17.23           O
ATOM    434  CB  VAL A  70      19.395  12.866  19.999  1.00 17.54           C
ATOM    435  CG1 VAL A  70      20.624  13.402  20.704  1.00 19.07           C
ATOM    436  CG2 VAL A  70      18.451  13.994  19.599  1.00 17.50           C
ATOM    437  N   TYR A  71      18.715  10.764  17.028  1.00 19.22           N
ATOM    438  CA  TYR A  71      17.615  10.071  16.367  1.00 19.79           C
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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 439 | C | TYR | A | 71 | 16.934 | 9.072 | 17.306 | 1.00 | 19.62 | C |
| ATOM | 440 | O | TYR | A | 71 | 15.726 | 9.120 | 17.457 | 1.00 | 18.64 | O |
| ATOM | 441 | CB | TYR | A | 71 | 18.082 | 9.406 | 15.055 | 1.00 | 20.19 | C |
| ATOM | 442 | CG | TYR | A | 71 | 17.156 | 8.320 | 14.554 | 1.00 | 22.29 | C |
| ATOM | 443 | CD1 | TYR | A | 71 | 15.938 | 8.619 | 13.948 | 1.00 | 25.33 | C |
| ATOM | 444 | CD2 | TYR | A | 71 | 17.503 | 6.986 | 14.691 | 1.00 | 23.31 | C |
| ATOM | 445 | CE1 | TYR | A | 71 | 15.080 | 7.555 | 13.480 | 1.00 | 24.74 | C |
| ATOM | 446 | CE2 | TYR | A | 71 | 16.684 | 5.968 | 14.252 | 1.00 | 23.57 | C |
| ATOM | 447 | CZ | TYR | A | 71 | 15.479 | 6.244 | 13.650 | 1.00 | 24.07 | C |
| ATOM | 448 | OH | TYR | A | 71 | 14.686 | 5.159 | 13.266 | 1.00 | 27.86 | O |
| ATOM | 449 | N | PRO | A | 72 | 17.688 | 8.200 | 17.960 | 1.00 | 20.27 | N |
| ATOM | 450 | CA | PRO | A | 72 | 17.074 | 7.196 | 18.840 | 1.00 | 21.30 | C |
| ATOM | 451 | C | PRO | A | 72 | 16.307 | 7.794 | 20.008 | 1.00 | 21.82 | C |
| ATOM | 452 | O | PRO | A | 72 | 15.463 | 7.120 | 20.535 | 1.00 | 21.13 | O |
| ATOM | 453 | CB | PRO | A | 72 | 18.267 | 6.377 | 19.351 | 1.00 | 21.33 | C |
| ATOM | 454 | CG | PRO | A | 72 | 19.362 | 6.650 | 18.386 | 1.00 | 21.75 | C |
| ATOM | 455 | CD | PRO | A | 72 | 19.151 | 8.065 | 17.905 | 1.00 | 20.71 | C |
| ATOM | 456 | N | ALA | A | 73 | 16.588 | 9.038 | 20.391 | 1.00 | 22.47 | N |
| ATOM | 457 | CA | ALA | A | 73 | 15.892 | 9.658 | 21.522 | 1.00 | 23.20 | C |
| ATOM | 458 | C | ALA | A | 73 | 14.567 | 10.293 | 21.103 | 1.00 | 23.47 | C |
| ATOM | 459 | O | ALA | A | 73 | 13.801 | 10.765 | 21.938 | 1.00 | 23.46 | O |
| ATOM | 460 | CB | ALA | A | 73 | 16.783 | 10.718 | 22.173 | 1.00 | 23.27 | C |
| ATOM | 461 | N | LEU | A | 74 | 14.297 | 10.322 | 19.808 | 1.00 | 23.79 | N |
| ATOM | 462 | CA | LEU | A | 74 | 13.086 | 10.967 | 19.329 | 1.00 | 24.10 | C |
| ATOM | 463 | C | LEU | A | 74 | 11.797 | 10.301 | 19.801 | 1.00 | 24.55 | C |
| ATOM | 464 | O | LEU | A | 74 | 10.732 | 10.903 | 19.746 | 1.00 | 23.83 | O |
| ATOM | 465 | CB | LEU | A | 74 | 13.114 | 11.076 | 17.810 | 1.00 | 24.16 | C |
| ATOM | 466 | CG | LEU | A | 74 | 14.185 | 12.061 | 17.296 | 1.00 | 24.67 | C |
| ATOM | 467 | CD1 | LEU | A | 74 | 13.988 | 12.320 | 15.820 | 1.00 | 26.73 | C |
| ATOM | 468 | CD2 | LEU | A | 74 | 14.225 | 13.371 | 18.077 | 1.00 | 23.39 | C |
| ATOM | 469 | N | LYS | A | 75 | 11.897 | 9.053 | 20.244 | 1.00 | 24.97 | N |
| ATOM | 470 | CA | LYS | A | 75 | 10.741 | 8.317 | 20.738 | 1.00 | 25.16 | C |
| ATOM | 471 | C | LYS | A | 75 | 10.589 | 8.519 | 22.245 | 1.00 | 25.37 | C |
| ATOM | 472 | O | LYS | A | 75 | 9.612 | 8.082 | 22.822 | 1.00 | 25.23 | O |
| ATOM | 473 | CB | LYS | A | 75 | 10.885 | 6.819 | 20.428 | 1.00 | 25.16 | C |
| ATOM | 474 | CG | LYS | A | 75 | 12.079 | 6.163 | 21.097 | 1.00 | 25.17 | C |
| ATOM | 475 | CD | LYS | A | 75 | 12.178 | 4.653 | 20.765 | 1.00 | 27.19 | C |
| ATOM | 476 | CE | LYS | A | 75 | 13.646 | 4.220 | 20.609 | 1.00 | 26.95 | C |
| ATOM | 477 | NZ | LYS | A | 75 | 14.348 | 4.123 | 21.868 | 1.00 | 26.22 | N |
| ATOM | 478 | N | TRP | A | 76 | 11.552 | 9.179 | 22.882 | 1.00 | 25.25 | N |
| ATOM | 479 | CA | TRP | A | 76 | 11.486 | 9.389 | 24.319 | 1.00 | 25.56 | C |
| ATOM | 480 | C | TRP | A | 76 | 10.268 | 10.201 | 24.749 | 1.00 | 26.35 | C |
| ATOM | 481 | O | TRP | A | 76 | 9.920 | 11.198 | 24.130 | 1.00 | 26.71 | O |
| ATOM | 482 | CB | TRP | A | 76 | 12.719 | 10.139 | 24.816 | 1.00 | 25.19 | C |
| ATOM | 483 | CG | TRP | A | 76 | 13.975 | 9.338 | 24.816 | 1.00 | 24.32 | C |
| ATOM | 484 | CD1 | TRP | A | 76 | 14.129 | 8.059 | 24.393 | 1.00 | 22.72 | C |
| ATOM | 485 | CD2 | TRP | A | 76 | 15.258 | 9.762 | 25.271 | 1.00 | 22.34 | C |
| ATOM | 486 | NE1 | TRP | A | 76 | 15.431 | 7.658 | 24.552 | 1.00 | 20.61 | N |
| ATOM | 487 | CE2 | TRP | A | 76 | 16.145 | 8.685 | 25.096 | 1.00 | 20.28 | C |
| ATOM | 488 | CE3 | TRP | A | 76 | 15.750 | 10.944 | 25.817 | 1.00 | 22.65 | C |
| ATOM | 489 | CZ2 | TRP | A | 76 | 17.481 | 8.756 | 25.437 | 1.00 | 20.18 | C |
| ATOM | 490 | CZ3 | TRP | A | 76 | 17.088 | 11.012 | 26.163 | 1.00 | 21.43 | C |
| ATOM | 491 | CH2 | TRP | A | 76 | 17.932 | 9.934 | 25.970 | 1.00 | 21.94 | C |
| ATOM | 492 | N | ASP | A | 77 | 9.643 | 9.772 | 25.836 | 1.00 | 26.46 | N |
| ATOM | 493 | CA | ASP | A | 77 | 8.583 | 10.530 | 26.467 | 1.00 | 26.47 | C |
| ATOM | 494 | C | ASP | A | 77 | 8.618 | 10.116 | 27.931 | 1.00 | 26.16 | C |
| ATOM | 495 | O | ASP | A | 77 | 9.405 | 9.264 | 28.291 | 1.00 | 26.44 | O |
| ATOM | 496 | CB | ASP | A | 77 | 7.230 | 10.276 | 25.810 | 1.00 | 26.51 | C |
| ATOM | 497 | CG | ASP | A | 77 | 6.795 | 8.835 | 25.885 | 1.00 | 27.32 | C |
| ATOM | 498 | OD1 | ASP | A | 77 | 7.388 | 8.015 | 26.638 | 1.00 | 26.02 | O |
| ATOM | 499 | OD2 | ASP | A | 77 | 5.832 | 8.439 | 25.211 | 1.00 | 29.97 | O |

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ATOM    500  N   LEU A  78       7.790  10.705  28.775  1.00 25.96           N
ATOM    501  CA  LEU A  78       7.893  10.441  30.201  1.00 26.27           C
ATOM    502  C   LEU A  78       7.716   8.965  30.539  1.00 26.14           C
ATOM    503  O   LEU A  78       8.446   8.438  31.374  1.00 25.51           O
ATOM    504  CB  LEU A  78       6.905  11.301  30.979  1.00 26.32           C
ATOM    505  CG  LEU A  78       7.155  12.802  30.860  1.00 27.35           C
ATOM    506  CD1 LEU A  78       6.098  13.579  31.623  1.00 28.05           C
ATOM    507  CD2 LEU A  78       8.536  13.165  31.379  1.00 28.39           C
ATOM    508  N   GLU A  79       6.775   8.297  29.874  1.00 26.56           N
ATOM    509  CA  GLU A  79       6.526   6.876  30.123  1.00 27.00           C
ATOM    510  C   GLU A  79       7.754   6.029  29.780  1.00 26.63           C
ATOM    511  O   GLU A  79       8.220   5.231  30.583  1.00 25.94           O
ATOM    512  CB  GLU A  79       5.302   6.371  29.333  1.00 27.39           C
ATOM    513  CG  GLU A  79       4.963   4.919  29.657  1.00 29.75           C
ATOM    514  CD  GLU A  79       3.803   4.347  28.854  1.00 33.15           C
ATOM    515  OE1 GLU A  79       3.361   4.976  27.863  1.00 35.39           O
ATOM    516  OE2 GLU A  79       3.338   3.245  29.224  1.00 35.44           O
ATOM    517  N   TYR A  80       8.279   6.205  28.575  1.00 26.53           N
ATOM    518  CA  TYR A  80       9.466   5.465  28.169  1.00 26.29           C
ATOM    519  C   TYR A  80      10.669   5.763  29.072  1.00 25.83           C
ATOM    520  O   TYR A  80      11.418   4.863  29.435  1.00 25.75           O
ATOM    521  CB  TYR A  80       9.812   5.802  26.728  1.00 26.53           C
ATOM    522  CG  TYR A  80      11.047   5.106  26.210  1.00 26.94           C
ATOM    523  CD1 TYR A  80      10.971   3.836  25.637  1.00 26.53           C
ATOM    524  CD2 TYR A  80      12.287   5.721  26.291  1.00 25.32           C
ATOM    525  CE1 TYR A  80      12.113   3.208  25.142  1.00 26.28           C
ATOM    526  CE2 TYR A  80      13.416   5.109  25.823  1.00 25.73           C
ATOM    527  CZ  TYR A  80      13.331   3.861  25.240  1.00 25.94           C
ATOM    528  OH  TYR A  80      14.478   3.294  24.758  1.00 25.55           O
ATOM    529  N   LEU A  81      10.859   7.016  29.448  1.00 25.62           N
ATOM    530  CA  LEU A  81      12.000   7.350  30.309  1.00 25.87           C
ATOM    531  C   LEU A  81      11.821   6.794  31.733  1.00 26.06           C
ATOM    532  O   LEU A  81      12.763   6.263  32.327  1.00 26.00           O
ATOM    533  CB  LEU A  81      12.250   8.863  30.340  1.00 25.81           C
ATOM    534  CG  LEU A  81      12.748   9.501  29.030  1.00 25.65           C
ATOM    535  CD1 LEU A  81      12.828  11.010  29.174  1.00 26.40           C
ATOM    536  CD2 LEU A  81      14.102   8.959  28.592  1.00 25.79           C
ATOM    537  N   GLN A  82      10.617   6.913  32.274  1.00 26.27           N
ATOM    538  CA  GLN A  82      10.338   6.388  33.602  1.00 26.77           C
ATOM    539  C   GLN A  82      10.640   4.897  33.623  1.00 26.51           C
ATOM    540  O   GLN A  82      11.232   4.384  34.552  1.00 26.60           O
ATOM    541  CB  GLN A  82       8.877   6.611  33.974  1.00 26.90           C
ATOM    542  CG  GLN A  82       8.466   5.856  35.236  1.00 28.41           C
ATOM    543  CD  GLN A  82       7.315   6.501  35.987  1.00 30.63           C
ATOM    544  OE1 GLN A  82       6.755   7.501  35.551  1.00 32.13           O
ATOM    545  NE2 GLN A  82       6.944   5.907  37.116  1.00 34.12           N
ATOM    546  N   GLU A  83      10.252   4.216  32.561  1.00 26.68           N
ATOM    547  CA  GLU A  83      10.429   2.773  32.456  1.00 26.90           C
ATOM    548  C   GLU A  83      11.893   2.359  32.295  1.00 26.42           C
ATOM    549  O   GLU A  83      12.285   1.294  32.764  1.00 25.50           O
ATOM    550  CB  GLU A  83       9.604   2.257  31.273  1.00 26.84           C
ATOM    551  CG  GLU A  83       9.607   0.753  31.080  1.00 29.20           C
ATOM    552  CD  GLU A  83       8.902   0.014  32.205  1.00 31.92           C
ATOM    553  OE1 GLU A  83       8.258   0.666  33.060  1.00 34.06           O
ATOM    554  OE2 GLU A  83       9.008  -1.221  32.243  1.00 33.78           O
ATOM    555  N   ASN A  84      12.711   3.223  31.700  1.00 25.79           N
ATOM    556  CA  ASN A  84      14.063   2.824  31.312  1.00 25.87           C
ATOM    557  C   ASN A  84      15.273   3.607  31.810  1.00 26.08           C
ATOM    558  O   ASN A  84      16.392   3.138  31.628  1.00 26.05           O
ATOM    559  CB  ASN A  84      14.137   2.844  29.784  1.00 25.74           C
ATOM    560  CG  ASN A  84      13.262   1.799  29.152  1.00 25.67           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 561 | OD1 | ASN | A | 84 | 13.402 | 0.608 | 29.439 | 1.00 | 24.26 | O |
| ATOM | 562 | ND2 | ASN | A | 84 | 12.354 | 2.231 | 28.288 | 1.00 | 22.66 | N |
| ATOM | 563 | N | ILE | A | 85 | 15.087 | 4.773 | 32.422 | 1.00 | 26.02 | N |
| ATOM | 564 | CA | ILE | A | 85 | 16.240 | 5.599 | 32.763 | 1.00 | 26.74 | C |
| ATOM | 565 | C | ILE | A | 85 | 16.930 | 5.307 | 34.099 | 1.00 | 26.89 | C |
| ATOM | 566 | O | ILE | A | 85 | 17.820 | 6.054 | 34.519 | 1.00 | 26.93 | O |
| ATOM | 567 | CB | ILE | A | 85 | 15.846 | 7.076 | 32.688 | 1.00 | 26.70 | C |
| ATOM | 568 | CG1 | ILE | A | 85 | 17.049 | 7.923 | 32.270 | 1.00 | 27.99 | C |
| ATOM | 569 | CG2 | ILE | A | 85 | 15.232 | 7.535 | 33.988 | 1.00 | 26.50 | C |
| ATOM | 570 | CD1 | ILE | A | 85 | 16.696 | 9.389 | 32.000 | 1.00 | 28.77 | C |
| ATOM | 571 | N | GLY | A | 86 | 16.503 | 4.253 | 34.773 | 1.00 | 27.27 | N |
| ATOM | 572 | CA | GLY | A | 86 | 17.130 | 3.834 | 36.018 | 1.00 | 27.51 | C |
| ATOM | 573 | C | GLY | A | 86 | 16.573 | 4.453 | 37.289 | 1.00 | 27.73 | C |
| ATOM | 574 | O | GLY | A | 86 | 15.563 | 5.163 | 37.268 | 1.00 | 27.80 | O |
| ATOM | 575 | N | ASN | A | 87 | 17.273 | 4.186 | 38.392 | 1.00 | 27.70 | N |
| ATOM | 576 | CA | ASN | A | 87 | 16.864 | 4.603 | 39.726 | 1.00 | 27.53 | C |
| ATOM | 577 | C | ASN | A | 87 | 17.849 | 5.602 | 40.320 | 1.00 | 27.33 | C |
| ATOM | 578 | O | ASN | A | 87 | 17.932 | 5.762 | 41.539 | 1.00 | 26.97 | O |
| ATOM | 579 | CB | ASN | A | 87 | 16.726 | 3.367 | 40.644 | 1.00 | 27.60 | C |
| ATOM | 580 | N | GLY | A | 88 | 18.601 | 6.273 | 39.455 | 1.00 | 27.41 | N |
| ATOM | 581 | CA | GLY | A | 88 | 19.528 | 7.307 | 39.888 | 1.00 | 27.29 | C |
| ATOM | 582 | C | GLY | A | 88 | 18.762 | 8.549 | 40.288 | 1.00 | 27.18 | C |
| ATOM | 583 | O | GLY | A | 88 | 17.570 | 8.654 | 40.001 | 1.00 | 27.43 | O |
| ATOM | 584 | N | ASP | A | 89 | 19.437 | 9.489 | 40.945 | 1.00 | 27.04 | N |
| ATOM | 585 | CA | ASP | A | 89 | 18.808 | 10.739 | 41.366 | 1.00 | 26.88 | C |
| ATOM | 586 | C | ASP | A | 89 | 18.761 | 11.755 | 40.227 | 1.00 | 26.69 | C |
| ATOM | 587 | O | ASP | A | 89 | 19.697 | 11.848 | 39.446 | 1.00 | 26.91 | O |
| ATOM | 588 | CB | ASP | A | 89 | 19.596 | 11.372 | 42.504 | 1.00 | 26.95 | C |
| ATOM | 589 | CG | ASP | A | 89 | 19.375 | 10.688 | 43.834 | 1.00 | 27.28 | C |
| ATOM | 590 | OD1 | ASP | A | 89 | 18.499 | 9.811 | 43.939 | 1.00 | 29.31 | O |
| ATOM | 591 | OD2 | ASP | A | 89 | 20.040 | 10.983 | 44.839 | 1.00 | 27.32 | O |
| ATOM | 592 | N | PHE | A | 90 | 17.687 | 12.531 | 40.152 | 1.00 | 26.24 | N |
| ATOM | 593 | CA | PHE | A | 90 | 17.598 | 13.594 | 39.165 | 1.00 | 26.10 | C |
| ATOM | 594 | C | PHE | A | 90 | 17.407 | 14.931 | 39.866 | 1.00 | 26.23 | C |
| ATOM | 595 | O | PHE | A | 90 | 16.629 | 15.037 | 40.811 | 1.00 | 26.48 | O |
| ATOM | 596 | CB | PHE | A | 90 | 16.460 | 13.322 | 38.184 | 1.00 | 25.91 | C |
| ATOM | 597 | CG | PHE | A | 90 | 16.747 | 12.201 | 37.241 | 1.00 | 25.26 | C |
| ATOM | 598 | CD1 | PHE | A | 90 | 16.601 | 10.886 | 37.640 | 1.00 | 25.32 | C |
| ATOM | 599 | CD2 | PHE | A | 90 | 17.190 | 12.459 | 35.958 | 1.00 | 26.02 | C |
| ATOM | 600 | CE1 | PHE | A | 90 | 16.872 | 9.856 | 36.777 | 1.00 | 24.09 | C |
| ATOM | 601 | CE2 | PHE | A | 90 | 17.460 | 11.427 | 35.091 | 1.00 | 25.07 | C |
| ATOM | 602 | CZ | PHE | A | 90 | 17.308 | 10.117 | 35.512 | 1.00 | 24.67 | C |
| ATOM | 603 | N | SER | A | 91 | 18.149 | 15.941 | 39.430 | 1.00 | 26.33 | N |
| ATOM | 604 | CA | SER | A | 91 | 17.985 | 17.280 | 39.973 | 1.00 | 26.48 | C |
| ATOM | 605 | C | SER | A | 91 | 16.777 | 17.923 | 39.310 | 1.00 | 26.71 | C |
| ATOM | 606 | O | SER | A | 91 | 16.696 | 18.029 | 38.077 | 1.00 | 26.09 | O |
| ATOM | 607 | CB | SER | A | 91 | 19.226 | 18.152 | 39.763 | 1.00 | 26.25 | C |
| ATOM | 608 | OG | SER | A | 91 | 20.364 | 17.543 | 40.326 | 1.00 | 26.61 | O |
| ATOM | 609 | N | VAL | A | 92 | 15.835 | 18.327 | 40.150 | 1.00 | 27.06 | N |
| ATOM | 610 | CA | VAL | A | 92 | 14.629 | 18.971 | 39.695 | 1.00 | 27.44 | C |
| ATOM | 611 | C | VAL | A | 92 | 14.468 | 20.295 | 40.405 | 1.00 | 27.57 | C |
| ATOM | 612 | O | VAL | A | 92 | 14.475 | 20.376 | 41.642 | 1.00 | 26.69 | O |
| ATOM | 613 | CB | VAL | A | 92 | 13.407 | 18.132 | 40.004 | 1.00 | 27.60 | C |
| ATOM | 614 | CG1 | VAL | A | 92 | 12.164 | 18.800 | 39.432 | 1.00 | 28.15 | C |
| ATOM | 615 | CG2 | VAL | A | 92 | 13.584 | 16.731 | 39.457 | 1.00 | 27.84 | C |
| ATOM | 616 | N | TYR | A | 93 | 14.312 | 21.334 | 39.598 | 1.00 | 27.77 | N |
| ATOM | 617 | CA | TYR | A | 93 | 14.120 | 22.661 | 40.108 | 1.00 | 27.91 | C |
| ATOM | 618 | C | TYR | A | 93 | 12.654 | 22.940 | 40.172 | 1.00 | 28.16 | C |
| ATOM | 619 | O | TYR | A | 93 | 11.894 | 22.525 | 39.303 | 1.00 | 28.02 | O |
| ATOM | 620 | CB | TYR | A | 93 | 14.810 | 23.673 | 39.216 | 1.00 | 27.94 | C |
| ATOM | 621 | CG | TYR | A | 93 | 16.291 | 23.593 | 39.368 | 1.00 | 29.53 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 622 | CD1 | TYR | A | 93 | 16.929 | 24.258 | 40.395 | 1.00 | 29.48 | C |
| ATOM | 623 | CD2 | TYR | A | 93 | 17.046 | 22.815 | 38.522 | 1.00 | 30.95 | C |
| ATOM | 624 | CE1 | TYR | A | 93 | 18.266 | 24.169 | 40.553 | 1.00 | 29.93 | C |
| ATOM | 625 | CE2 | TYR | A | 93 | 18.386 | 22.726 | 38.679 | 1.00 | 31.90 | C |
| ATOM | 626 | CZ | TYR | A | 93 | 18.985 | 23.402 | 39.704 | 1.00 | 31.56 | C |
| ATOM | 627 | OH | TYR | A | 93 | 20.327 | 23.306 | 39.878 | 1.00 | 35.47 | O |
| ATOM | 628 | N | SER | A | 94 | 12.282 | 23.669 | 41.208 | 1.00 | 28.70 | N |
| ATOM | 629 | CA | SER | A | 94 | 10.913 | 24.037 | 41.459 | 1.00 | 29.47 | C |
| ATOM | 630 | C | SER | A | 94 | 10.856 | 25.547 | 41.554 | 1.00 | 29.69 | C |
| ATOM | 631 | O | SER | A | 94 | 11.705 | 26.167 | 42.187 | 1.00 | 29.50 | O |
| ATOM | 632 | CB | SER | A | 94 | 10.456 | 23.411 | 42.774 | 1.00 | 29.32 | C |
| ATOM | 633 | OG | SER | A | 94 | 9.093 | 23.701 | 43.009 | 1.00 | 30.85 | O |
| ATOM | 634 | N | ALA | A | 95 | 9.858 | 26.146 | 40.928 | 1.00 | 30.39 | N |
| ATOM | 635 | CA | ALA | A | 95 | 9.760 | 27.591 | 40.929 | 1.00 | 31.04 | C |
| ATOM | 636 | C | ALA | A | 95 | 8.330 | 28.064 | 40.932 | 1.00 | 31.76 | C |
| ATOM | 637 | O | ALA | A | 95 | 7.425 | 27.386 | 40.452 | 1.00 | 31.87 | O |
| ATOM | 638 | CB | ALA | A | 95 | 10.480 | 28.165 | 39.716 | 1.00 | 31.12 | C |
| ATOM | 639 | N | SER | A | 96 | 8.147 | 29.258 | 41.467 | 1.00 | 32.54 | N |
| ATOM | 640 | CA | SER | A | 96 | 6.848 | 29.891 | 41.489 | 1.00 | 33.42 | C |
| ATOM | 641 | C | SER | A | 96 | 6.708 | 30.869 | 40.326 | 1.00 | 33.15 | C |
| ATOM | 642 | O | SER | A | 96 | 5.662 | 31.487 | 40.163 | 1.00 | 34.35 | O |
| ATOM | 643 | CB | SER | A | 96 | 6.673 | 30.661 | 42.787 | 1.00 | 33.88 | C |
| ATOM | 644 | OG | SER | A | 96 | 5.380 | 31.217 | 42.815 | 1.00 | 35.79 | O |
| ATOM | 645 | N | THR | A | 97 | 7.775 | 31.031 | 39.554 | 1.00 | 32.09 | N |
| ATOM | 646 | CA | THR | A | 97 | 7.797 | 31.920 | 38.397 | 1.00 | 31.44 | C |
| ATOM | 647 | C | THR | A | 97 | 8.185 | 31.095 | 37.191 | 1.00 | 30.26 | C |
| ATOM | 648 | O | THR | A | 97 | 8.693 | 30.003 | 37.348 | 1.00 | 29.72 | O |
| ATOM | 649 | CB | THR | A | 97 | 8.857 | 33.031 | 38.582 | 1.00 | 31.64 | C |
| ATOM | 650 | OG1 | THR | A | 97 | 9.147 | 33.656 | 37.323 | 1.00 | 32.17 | O |
| ATOM | 651 | CG2 | THR | A | 97 | 10.227 | 32.455 | 38.978 | 1.00 | 31.73 | C |
| ATOM | 652 | N | HIS | A | 98 | 7.974 | 31.623 | 35.996 | 1.00 | 29.35 | N |
| ATOM | 653 | CA | HIS | A | 98 | 8.379 | 30.915 | 34.780 | 1.00 | 28.83 | C |
| ATOM | 654 | C | HIS | A | 98 | 9.899 | 30.969 | 34.589 | 1.00 | 28.37 | C |
| ATOM | 655 | O | HIS | A | 98 | 10.467 | 30.189 | 33.824 | 1.00 | 27.53 | O |
| ATOM | 656 | CB | HIS | A | 98 | 7.671 | 31.490 | 33.548 | 1.00 | 28.76 | C |
| ATOM | 657 | CG | HIS | A | 98 | 7.936 | 32.942 | 33.309 | 1.00 | 28.53 | C |
| ATOM | 658 | ND1 | HIS | A | 98 | 7.271 | 33.944 | 33.984 | 1.00 | 29.18 | N |
| ATOM | 659 | CD2 | HIS | A | 98 | 8.793 | 33.566 | 32.463 | 1.00 | 29.68 | C |
| ATOM | 660 | CE1 | HIS | A | 98 | 7.708 | 35.120 | 33.568 | 1.00 | 29.42 | C |
| ATOM | 661 | NE2 | HIS | A | 98 | 8.638 | 34.919 | 32.650 | 1.00 | 29.10 | N |
| ATOM | 662 | N | LYS | A | 99 | 10.562 | 31.874 | 35.299 | 1.00 | 27.85 | N |
| ATOM | 663 | CA | LYS | A | 99 | 11.997 | 32.041 | 35.124 | 1.00 | 28.24 | C |
| ATOM | 664 | C | LYS | A | 99 | 12.878 | 31.143 | 35.997 | 1.00 | 27.69 | C |
| ATOM | 665 | O | LYS | A | 99 | 12.892 | 31.278 | 37.216 | 1.00 | 29.10 | O |
| ATOM | 666 | CB | LYS | A | 99 | 12.366 | 33.498 | 35.349 | 1.00 | 28.47 | C |
| ATOM | 667 | CG | LYS | A | 99 | 11.836 | 34.410 | 34.255 | 1.00 | 30.42 | C |
| ATOM | 668 | CD | LYS | A | 99 | 12.431 | 35.791 | 34.347 | 1.00 | 32.66 | C |
| ATOM | 669 | CE | LYS | A | 99 | 11.757 | 36.624 | 35.421 | 1.00 | 34.45 | C |
| ATOM | 670 | NZ | LYS | A | 99 | 10.569 | 37.347 | 34.884 | 1.00 | 35.39 | N |
| ATOM | 671 | N | PHE | A | 100 | 13.621 | 30.237 | 35.376 | 1.00 | 26.40 | N |
| ATOM | 672 | CA | PHE | A | 100 | 14.551 | 29.397 | 36.127 | 1.00 | 25.95 | C |
| ATOM | 673 | C | PHE | A | 100 | 15.978 | 29.920 | 35.995 | 1.00 | 25.87 | C |
| ATOM | 674 | O | PHE | A | 100 | 16.809 | 29.386 | 35.247 | 1.00 | 25.86 | O |
| ATOM | 675 | CB | PHE | A | 100 | 14.469 | 27.945 | 35.686 | 1.00 | 25.48 | C |
| ATOM | 676 | CG | PHE | A | 100 | 13.211 | 27.267 | 36.109 | 1.00 | 25.06 | C |
| ATOM | 677 | CD1 | PHE | A | 100 | 12.047 | 27.436 | 35.388 | 1.00 | 24.80 | C |
| ATOM | 678 | CD2 | PHE | A | 100 | 13.191 | 26.472 | 37.238 | 1.00 | 25.18 | C |
| ATOM | 679 | CE1 | PHE | A | 100 | 10.886 | 26.805 | 35.772 | 1.00 | 25.96 | C |
| ATOM | 680 | CE2 | PHE | A | 100 | 12.030 | 25.835 | 37.631 | 1.00 | 25.79 | C |
| ATOM | 681 | CZ | PHE | A | 100 | 10.878 | 26.004 | 36.898 | 1.00 | 26.05 | C |
| ATOM | 682 | N | LEU | A | 101 | 16.237 | 30.997 | 36.709 | 1.00 | 25.77 | N |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 683 | CA | LEU A 101 | 17.549 | 31.589 | 36.747 | 1.00 | 25.85 | C |
| ATOM | 684 | C | LEU A 101 | 18.527 | 30.605 | 37.381 | 1.00 | 25.87 | C |
| ATOM | 685 | O | LEU A 101 | 18.319 | 30.136 | 38.503 | 1.00 | 24.99 | O |
| ATOM | 686 | CB | LEU A 101 | 17.488 | 32.876 | 37.559 | 1.00 | 25.84 | C |
| ATOM | 687 | CG | LEU A 101 | 18.795 | 33.656 | 37.708 | 1.00 | 26.07 | C |
| ATOM | 688 | CD1 | LEU A 101 | 19.244 | 34.200 | 36.377 | 1.00 | 25.11 | C |
| ATOM | 689 | CD2 | LEU A 101 | 18.609 | 34.800 | 38.710 | 1.00 | 27.75 | C |
| ATOM | 690 | N | TYR A 102 | 19.582 | 30.274 | 36.644 | 1.00 | 26.56 | N |
| ATOM | 691 | CA | TYR A 102 | 20.611 | 29.380 | 37.159 | 1.00 | 26.99 | C |
| ATOM | 692 | C | TYR A 102 | 21.430 | 30.072 | 38.260 | 1.00 | 27.10 | C |
| ATOM | 693 | O | TYR A 102 | 21.711 | 31.264 | 38.174 | 1.00 | 27.00 | O |
| ATOM | 694 | CB | TYR A 102 | 21.562 | 28.939 | 36.053 | 1.00 | 27.26 | C |
| ATOM | 695 | CG | TYR A 102 | 22.667 | 28.088 | 36.620 | 1.00 | 28.93 | C |
| ATOM | 696 | CD1 | TYR A 102 | 22.457 | 26.750 | 36.914 | 1.00 | 29.52 | C |
| ATOM | 697 | CD2 | TYR A 102 | 23.906 | 28.636 | 36.909 | 1.00 | 31.11 | C |
| ATOM | 698 | CE1 | TYR A 102 | 23.463 | 25.979 | 37.480 | 1.00 | 32.23 | C |
| ATOM | 699 | CE2 | TYR A 102 | 24.913 | 27.872 | 37.470 | 1.00 | 32.52 | C |
| ATOM | 700 | CZ | TYR A 102 | 24.693 | 26.549 | 37.750 | 1.00 | 33.88 | C |
| ATOM | 701 | OH | TYR A 102 | 25.727 | 25.794 | 38.314 | 1.00 | 38.68 | O |
| ATOM | 702 | N | TYR A 103 | 21.793 | 29.322 | 39.296 | 1.00 | 26.83 | N |
| ATOM | 703 | CA | TYR A 103 | 22.667 | 29.840 | 40.343 | 1.00 | 27.22 | C |
| ATOM | 704 | C | TYR A 103 | 23.613 | 28.750 | 40.834 | 1.00 | 26.77 | C |
| ATOM | 705 | O | TYR A 103 | 23.287 | 27.556 | 40.853 | 1.00 | 25.60 | O |
| ATOM | 706 | CB | TYR A 103 | 21.880 | 30.440 | 41.517 | 1.00 | 27.38 | C |
| ATOM | 707 | CG | TYR A 103 | 20.909 | 29.493 | 42.154 | 1.00 | 29.11 | C |
| ATOM | 708 | CD1 | TYR A 103 | 19.639 | 29.340 | 41.639 | 1.00 | 30.58 | C |
| ATOM | 709 | CD2 | TYR A 103 | 21.257 | 28.759 | 43.279 | 1.00 | 32.13 | C |
| ATOM | 710 | CE1 | TYR A 103 | 18.734 | 28.469 | 42.212 | 1.00 | 32.78 | C |
| ATOM | 711 | CE2 | TYR A 103 | 20.357 | 27.887 | 43.877 | 1.00 | 33.15 | C |
| ATOM | 712 | CZ | TYR A 103 | 19.096 | 27.745 | 43.329 | 1.00 | 34.41 | C |
| ATOM | 713 | OH | TYR A 103 | 18.187 | 26.888 | 43.892 | 1.00 | 37.44 | O |
| ATOM | 714 | N | ASP A 104 | 24.798 | 29.182 | 41.225 | 1.00 | 26.36 | N |
| ATOM | 715 | CA | ASP A 104 | 25.832 | 28.273 | 41.673 | 1.00 | 26.28 | C |
| ATOM | 716 | C | ASP A 104 | 25.802 | 28.239 | 43.184 | 1.00 | 26.21 | C |
| ATOM | 717 | O | ASP A 104 | 26.163 | 29.212 | 43.845 | 1.00 | 25.45 | O |
| ATOM | 718 | CB | ASP A 104 | 27.174 | 28.765 | 41.154 | 1.00 | 25.92 | C |
| ATOM | 719 | CG | ASP A 104 | 28.330 | 27.889 | 41.575 | 1.00 | 27.39 | C |
| ATOM | 720 | OD1 | ASP A 104 | 28.161 | 26.973 | 42.437 | 1.00 | 27.13 | O |
| ATOM | 721 | OD2 | ASP A 104 | 29.459 | 28.068 | 41.075 | 1.00 | 27.68 | O |
| ATOM | 722 | N | GLU A 105 | 25.358 | 27.114 | 43.724 | 1.00 | 26.46 | N |
| ATOM | 723 | CA | GLU A 105 | 25.218 | 26.962 | 45.162 | 1.00 | 27.02 | C |
| ATOM | 724 | C | GLU A 105 | 26.540 | 27.199 | 45.916 | 1.00 | 26.91 | C |
| ATOM | 725 | O | GLU A 105 | 26.523 | 27.718 | 47.026 | 1.00 | 26.51 | O |
| ATOM | 726 | CB | GLU A 105 | 24.602 | 25.587 | 45.481 | 1.00 | 27.45 | C |
| ATOM | 727 | CG | GLU A 105 | 23.088 | 25.556 | 45.254 | 1.00 | 29.46 | C |
| ATOM | 728 | CD | GLU A 105 | 22.527 | 24.158 | 45.025 | 1.00 | 32.85 | C |
| ATOM | 729 | OE1 | GLU A 105 | 22.908 | 23.234 | 45.765 | 1.00 | 32.90 | O |
| ATOM | 730 | OE2 | GLU A 105 | 21.703 | 23.980 | 44.085 | 1.00 | 35.16 | O |
| ATOM | 731 | N | LYS A 106 | 27.680 | 26.874 | 45.305 | 1.00 | 27.12 | N |
| ATOM | 732 | CA | LYS A 106 | 28.979 | 27.041 | 45.983 | 1.00 | 27.54 | C |
| ATOM | 733 | C | LYS A 106 | 29.331 | 28.493 | 46.258 | 1.00 | 27.70 | C |
| ATOM | 734 | O | LYS A 106 | 30.164 | 28.769 | 47.099 | 1.00 | 27.61 | O |
| ATOM | 735 | CB | LYS A 106 | 30.127 | 26.441 | 45.163 | 1.00 | 27.58 | C |
| ATOM | 736 | CG | LYS A 106 | 30.038 | 24.928 | 44.918 | 1.00 | 28.61 | C |
| ATOM | 737 | N | LYS A 107 | 28.713 | 29.420 | 45.537 | 1.00 | 27.99 | N |
| ATOM | 738 | CA | LYS A 107 | 29.020 | 30.826 | 45.694 | 1.00 | 28.30 | C |
| ATOM | 739 | C | LYS A 107 | 28.034 | 31.513 | 46.631 | 1.00 | 29.21 | C |
| ATOM | 740 | O | LYS A 107 | 28.175 | 32.701 | 46.917 | 1.00 | 29.08 | O |
| ATOM | 741 | CB | LYS A 107 | 29.040 | 31.524 | 44.324 | 1.00 | 28.30 | C |
| ATOM | 742 | CG | LYS A 107 | 30.344 | 31.291 | 43.516 | 1.00 | 28.07 | C |
| ATOM | 743 | CD | LYS A 107 | 30.242 | 31.737 | 42.034 | 1.00 | 27.29 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 744 | CE | LYS | A | 107 | 31.584 | 31.518 | 41.315 | 1.00 | 26.86 | C |
| ATOM | 745 | NZ | LYS | A | 107 | 31.642 | 31.889 | 39.870 | 1.00 | 24.80 | N |
| ATOM | 746 | N | MET | A | 108 | 27.041 | 30.781 | 47.125 | 1.00 | 30.08 | N |
| ATOM | 747 | CA | MET | A | 108 | 26.031 | 31.405 | 47.982 | 1.00 | 31.53 | C |
| ATOM | 748 | C | MET | A | 108 | 26.581 | 31.952 | 49.309 | 1.00 | 32.44 | C |
| ATOM | 749 | O | MET | A | 108 | 26.102 | 32.972 | 49.812 | 1.00 | 32.47 | O |
| ATOM | 750 | CB | MET | A | 108 | 24.862 | 30.452 | 48.218 | 1.00 | 31.81 | C |
| ATOM | 751 | CG | MET | A | 108 | 24.072 | 30.193 | 46.932 | 1.00 | 33.07 | C |
| ATOM | 752 | SD | MET | A | 108 | 22.625 | 29.140 | 47.064 | 1.00 | 35.76 | S |
| ATOM | 753 | CE | MET | A | 108 | 21.540 | 30.140 | 48.050 | 1.00 | 35.99 | C |
| ATOM | 754 | N | ALA | A | 109 | 27.603 | 31.315 | 49.860 | 1.00 | 33.56 | N |
| ATOM | 755 | CA | ALA | A | 109 | 28.154 | 31.769 | 51.138 | 1.00 | 34.94 | C |
| ATOM | 756 | C | ALA | A | 109 | 28.651 | 33.212 | 51.060 | 1.00 | 35.81 | C |
| ATOM | 757 | O | ALA | A | 109 | 28.483 | 33.989 | 51.991 | 1.00 | 36.23 | O |
| ATOM | 758 | CB | ALA | A | 109 | 29.279 | 30.838 | 51.606 | 1.00 | 34.82 | C |
| ATOM | 759 | N | ASN | A | 110 | 29.236 | 33.575 | 49.929 | 1.00 | 37.05 | N |
| ATOM | 760 | CA | ASN | A | 110 | 29.774 | 34.918 | 49.748 | 1.00 | 37.94 | C |
| ATOM | 761 | C | ASN | A | 110 | 28.731 | 35.992 | 49.413 | 1.00 | 38.13 | C |
| ATOM | 762 | O | ASN | A | 110 | 29.064 | 37.167 | 49.293 | 1.00 | 37.92 | O |
| ATOM | 763 | CB | ASN | A | 110 | 30.855 | 34.878 | 48.669 | 1.00 | 38.16 | C |
| ATOM | 764 | CG | ASN | A | 110 | 32.050 | 34.035 | 49.079 | 1.00 | 39.37 | C |
| ATOM | 765 | OD1 | ASN | A | 110 | 32.407 | 33.964 | 50.265 | 1.00 | 40.12 | O |
| ATOM | 766 | ND2 | ASN | A | 110 | 32.670 | 33.377 | 48.103 | 1.00 | 39.46 | N |
| ATOM | 767 | N | PHE | A | 111 | 27.480 | 35.588 | 49.234 | 1.00 | 38.71 | N |
| ATOM | 768 | CA | PHE | A | 111 | 26.408 | 36.539 | 48.966 | 1.00 | 39.02 | C |
| ATOM | 769 | C | PHE | A | 111 | 25.180 | 36.135 | 49.773 | 1.00 | 39.71 | C |
| ATOM | 770 | O | PHE | A | 111 | 24.143 | 35.747 | 49.232 | 1.00 | 39.45 | O |
| ATOM | 771 | CB | PHE | A | 111 | 26.091 | 36.603 | 47.471 | 1.00 | 38.97 | C |
| ATOM | 772 | CG | PHE | A | 111 | 27.110 | 37.362 | 46.672 | 1.00 | 38.04 | C |
| ATOM | 773 | CD1 | PHE | A | 111 | 28.329 | 36.791 | 46.363 | 1.00 | 37.99 | C |
| ATOM | 774 | CD2 | PHE | A | 111 | 26.851 | 38.642 | 46.235 | 1.00 | 36.83 | C |
| ATOM | 775 | CE1 | PHE | A | 111 | 29.269 | 37.493 | 45.635 | 1.00 | 37.68 | C |
| ATOM | 776 | CE2 | PHE | A | 111 | 27.788 | 39.339 | 45.500 | 1.00 | 36.08 | C |
| ATOM | 777 | CZ | PHE | A | 111 | 28.994 | 38.768 | 45.208 | 1.00 | 35.84 | C |
| ATOM | 778 | N | GLN | A | 112 | 25.315 | 36.267 | 51.085 | 1.00 | 40.62 | N |
| ATOM | 779 | CA | GLN | A | 112 | 24.286 | 35.852 | 52.029 | 1.00 | 41.31 | C |
| ATOM | 780 | C | GLN | A | 112 | 22.915 | 36.430 | 51.721 | 1.00 | 41.10 | C |
| ATOM | 781 | O | GLN | A | 112 | 21.906 | 35.827 | 52.060 | 1.00 | 41.31 | O |
| ATOM | 782 | CB | GLN | A | 112 | 24.701 | 36.236 | 53.451 | 1.00 | 41.65 | C |
| ATOM | 783 | CG | GLN | A | 112 | 26.058 | 35.694 | 53.882 | 1.00 | 43.80 | C |
| ATOM | 784 | CD | GLN | A | 112 | 26.104 | 34.177 | 53.938 | 1.00 | 46.42 | C |
| ATOM | 785 | OE1 | GLN | A | 112 | 25.394 | 33.501 | 53.191 | 1.00 | 48.56 | O |
| ATOM | 786 | NE2 | GLN | A | 112 | 26.951 | 33.637 | 54.816 | 1.00 | 46.94 | N |
| ATOM | 787 | N | ASN | A | 113 | 22.876 | 37.588 | 51.074 | 1.00 | 41.02 | N |
| ATOM | 788 | CA | ASN | A | 113 | 21.606 | 38.229 | 50.749 | 1.00 | 40.98 | C |
| ATOM | 789 | C | ASN | A | 113 | 20.954 | 37.760 | 49.440 | 1.00 | 40.71 | C |
| ATOM | 790 | O | ASN | A | 113 | 19.889 | 38.251 | 49.071 | 1.00 | 40.77 | O |
| ATOM | 791 | CB | ASN | A | 113 | 21.778 | 39.753 | 50.737 | 1.00 | 41.09 | C |
| ATOM | 792 | CG | ASN | A | 113 | 22.129 | 40.314 | 52.123 | 1.00 | 41.51 | C |
| ATOM | 793 | OD1 | ASN | A | 113 | 21.717 | 39.772 | 53.158 | 1.00 | 40.60 | O |
| ATOM | 794 | ND2 | ASN | A | 113 | 22.892 | 41.401 | 52.141 | 1.00 | 41.19 | N |
| ATOM | 795 | N | PHE | A | 114 | 21.571 | 36.826 | 48.725 | 1.00 | 40.34 | N |
| ATOM | 796 | CA | PHE | A | 114 | 20.934 | 36.321 | 47.515 | 1.00 | 39.86 | C |
| ATOM | 797 | C | PHE | A | 114 | 19.908 | 35.266 | 47.902 | 1.00 | 39.46 | C |
| ATOM | 798 | O | PHE | A | 114 | 20.235 | 34.299 | 48.584 | 1.00 | 38.82 | O |
| ATOM | 799 | CB | PHE | A | 114 | 21.940 | 35.714 | 46.552 | 1.00 | 39.96 | C |
| ATOM | 800 | CG | PHE | A | 114 | 21.298 | 35.059 | 45.362 | 1.00 | 40.54 | C |
| ATOM | 801 | CD1 | PHE | A | 114 | 20.670 | 35.828 | 44.395 | 1.00 | 40.29 | C |
| ATOM | 802 | CD2 | PHE | A | 114 | 21.295 | 33.679 | 45.224 | 1.00 | 40.62 | C |
| ATOM | 803 | CE1 | PHE | A | 114 | 20.061 | 35.237 | 43.307 | 1.00 | 40.20 | C |
| ATOM | 804 | CE2 | PHE | A | 114 | 20.684 | 33.082 | 44.126 | 1.00 | 40.36 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 805 | CZ | PHE | A | 114 | 20.066 | 33.866 | 43.172 | 1.00 | 40.52 | C |
| ATOM | 806 | N | LYS | A | 115 | 18.669 | 35.457 | 47.461 | 1.00 | 39.11 | N |
| ATOM | 807 | CA | LYS | A | 115 | 17.596 | 34.529 | 47.787 | 1.00 | 39.02 | C |
| ATOM | 808 | C | LYS | A | 115 | 17.042 | 33.938 | 46.497 | 1.00 | 38.71 | C |
| ATOM | 809 | O | LYS | A | 115 | 16.285 | 34.590 | 45.787 | 1.00 | 39.00 | O |
| ATOM | 810 | CB | LYS | A | 115 | 16.498 | 35.251 | 48.578 | 1.00 | 39.14 | C |
| ATOM | 811 | N | PRO | A | 116 | 17.389 | 32.691 | 46.213 | 1.00 | 38.17 | N |
| ATOM | 812 | CA | PRO | A | 116 | 17.027 | 32.060 | 44.938 | 1.00 | 37.95 | C |
| ATOM | 813 | C | PRO | A | 116 | 15.532 | 31.889 | 44.783 | 1.00 | 37.38 | C |
| ATOM | 814 | O | PRO | A | 116 | 14.865 | 31.506 | 45.733 | 1.00 | 37.36 | O |
| ATOM | 815 | CB | PRO | A | 116 | 17.684 | 30.679 | 45.004 | 1.00 | 38.15 | C |
| ATOM | 816 | CG | PRO | A | 116 | 18.416 | 30.604 | 46.297 | 1.00 | 38.40 | C |
| ATOM | 817 | CD | PRO | A | 116 | 18.079 | 31.775 | 47.125 | 1.00 | 38.19 | C |
| ATOM | 818 | N | ARG | A | 117 | 15.027 | 32.161 | 43.590 | 1.00 | 36.84 | N |
| ATOM | 819 | CA | ARG | A | 117 | 13.611 | 32.028 | 43.293 | 1.00 | 36.61 | C |
| ATOM | 820 | C | ARG | A | 117 | 13.259 | 30.581 | 42.984 | 1.00 | 36.38 | C |
| ATOM | 821 | O | ARG | A | 117 | 12.084 | 30.230 | 42.913 | 1.00 | 36.44 | O |
| ATOM | 822 | CB | ARG | A | 117 | 13.235 | 32.913 | 42.122 | 1.00 | 36.62 | C |
| ATOM | 823 | N | SER | A | 118 | 14.271 | 29.745 | 42.777 | 1.00 | 35.79 | N |
| ATOM | 824 | CA | SER | A | 118 | 14.025 | 28.339 | 42.538 | 1.00 | 35.51 | C |
| ATOM | 825 | C | SER | A | 118 | 14.844 | 27.491 | 43.512 | 1.00 | 35.35 | C |
| ATOM | 826 | O | SER | A | 118 | 15.888 | 27.923 | 43.991 | 1.00 | 35.16 | O |
| ATOM | 827 | CB | SER | A | 118 | 14.330 | 27.976 | 41.086 | 1.00 | 35.26 | C |
| ATOM | 828 | OG | SER | A | 118 | 15.689 | 28.164 | 40.795 | 1.00 | 35.14 | O |
| ATOM | 829 | N | ASN | A | 119 | 14.329 | 26.306 | 43.824 | 1.00 | 35.11 | N |
| ATOM | 830 | CA | ASN | A | 119 | 14.997 | 25.373 | 44.715 | 1.00 | 35.21 | C |
| ATOM | 831 | C | ASN | A | 119 | 15.233 | 24.049 | 44.022 | 1.00 | 34.26 | C |
| ATOM | 832 | O | ASN | A | 119 | 14.401 | 23.595 | 43.244 | 1.00 | 34.11 | O |
| ATOM | 833 | CB | ASN | A | 119 | 14.145 | 25.110 | 45.957 | 1.00 | 35.95 | C |
| ATOM | 834 | CG | ASN | A | 119 | 13.636 | 26.382 | 46.592 | 1.00 | 38.47 | C |
| ATOM | 835 | OD1 | ASN | A | 119 | 14.417 | 27.245 | 47.025 | 1.00 | 41.76 | O |
| ATOM | 836 | ND2 | ASN | A | 119 | 12.314 | 26.511 | 46.657 | 1.00 | 42.21 | N |
| ATOM | 837 | N | ARG | A | 120 | 16.368 | 23.434 | 44.326 | 1.00 | 33.75 | N |
| ATOM | 838 | CA | ARG | A | 120 | 16.750 | 22.149 | 43.761 | 1.00 | 33.33 | C |
| ATOM | 839 | C | ARG | A | 120 | 16.327 | 21.045 | 44.699 | 1.00 | 33.26 | C |
| ATOM | 840 | O | ARG | A | 120 | 16.523 | 21.138 | 45.910 | 1.00 | 33.07 | O |
| ATOM | 841 | CB | ARG | A | 120 | 18.270 | 22.075 | 43.592 | 1.00 | 33.37 | C |
| ATOM | 842 | CG | ARG | A | 120 | 18.759 | 20.889 | 42.771 | 1.00 | 32.70 | C |
| ATOM | 843 | CD | ARG | A | 120 | 20.277 | 20.732 | 42.743 | 1.00 | 31.64 | C |
| ATOM | 844 | NE | ARG | A | 120 | 20.892 | 21.165 | 43.992 | 1.00 | 31.16 | N |
| ATOM | 845 | CZ | ARG | A | 120 | 21.233 | 20.357 | 44.993 | 1.00 | 31.33 | C |
| ATOM | 846 | NH1 | ARG | A | 120 | 21.027 | 19.047 | 44.920 | 1.00 | 30.77 | N |
| ATOM | 847 | NH2 | ARG | A | 120 | 21.789 | 20.867 | 46.077 | 1.00 | 31.01 | N |
| ATOM | 848 | N | GLU | A | 121 | 15.735 | 20.001 | 44.137 | 1.00 | 32.98 | N |
| ATOM | 849 | CA | GLU | A | 121 | 15.379 | 18.827 | 44.904 | 1.00 | 32.85 | C |
| ATOM | 850 | C | GLU | A | 121 | 15.846 | 17.630 | 44.095 | 1.00 | 32.17 | C |
| ATOM | 851 | O | GLU | A | 121 | 15.744 | 17.612 | 42.864 | 1.00 | 32.36 | O |
| ATOM | 852 | CB | GLU | A | 121 | 13.874 | 18.767 | 45.179 | 1.00 | 33.21 | C |
| ATOM | 853 | CG | GLU | A | 121 | 13.420 | 17.468 | 45.826 | 1.00 | 35.39 | C |
| ATOM | 854 | CD | GLU | A | 121 | 12.189 | 17.629 | 46.699 | 1.00 | 38.11 | C |
| ATOM | 855 | OE1 | GLU | A | 121 | 12.326 | 18.152 | 47.830 | 1.00 | 41.26 | O |
| ATOM | 856 | OE2 | GLU | A | 121 | 11.091 | 17.221 | 46.270 | 1.00 | 39.55 | O |
| ATOM | 857 | N | GLU | A | 122 | 16.400 | 16.648 | 44.786 | 1.00 | 31.28 | N |
| ATOM | 858 | CA | GLU | A | 122 | 16.886 | 15.448 | 44.150 | 1.00 | 30.61 | C |
| ATOM | 859 | C | GLU | A | 122 | 15.814 | 14.392 | 44.298 | 1.00 | 30.31 | C |
| ATOM | 860 | O | GLU | A | 122 | 15.328 | 14.165 | 45.395 | 1.00 | 30.07 | O |
| ATOM | 861 | CB | GLU | A | 122 | 18.163 | 14.980 | 44.833 | 1.00 | 30.52 | C |
| ATOM | 862 | CG | GLU | A | 122 | 19.293 | 15.983 | 44.771 | 1.00 | 29.67 | C |
| ATOM | 863 | CD | GLU | A | 122 | 19.747 | 16.253 | 43.348 | 1.00 | 29.79 | C |
| ATOM | 864 | OE1 | GLU | A | 122 | 20.120 | 15.280 | 42.667 | 1.00 | 28.28 | O |
| ATOM | 865 | OE2 | GLU | A | 122 | 19.734 | 17.439 | 42.914 | 1.00 | 27.93 | O |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 866 | N | MET A 123 | 15.432 | 13.751 | 43.202 | 1.00 | 29.74 | N |
| ATOM | 867 | CA | MET A 123 | 14.407 | 12.728 | 43.277 | 1.00 | 29.77 | C |
| ATOM | 868 | C | MET A 123 | 14.594 | 11.683 | 42.202 | 1.00 | 29.31 | C |
| ATOM | 869 | O | MET A 123 | 15.408 | 11.842 | 41.294 | 1.00 | 29.42 | O |
| ATOM | 870 | CB | MET A 123 | 13.016 | 13.354 | 43.165 | 1.00 | 29.81 | C |
| ATOM | 871 | CG | MET A 123 | 12.749 | 14.057 | 41.865 | 1.00 | 30.27 | C |
| ATOM | 872 | SD | MET A 123 | 11.181 | 14.960 | 41.871 | 1.00 | 31.65 | S |
| ATOM | 873 | CE | MET A 123 | 11.582 | 16.371 | 42.804 | 1.00 | 31.47 | C |
| ATOM | 874 | N | LYS A 124 | 13.835 | 10.604 | 42.332 | 1.00 | 28.82 | N |
| ATOM | 875 | CA | LYS A 124 | 13.841 | 9.535 | 41.352 | 1.00 | 28.33 | C |
| ATOM | 876 | C | LYS A 124 | 12.959 | 9.976 | 40.191 | 1.00 | 27.51 | C |
| ATOM | 877 | O | LYS A 124 | 12.077 | 10.817 | 40.361 | 1.00 | 26.52 | O |
| ATOM | 878 | CB | LYS A 124 | 13.330 | 8.242 | 41.984 | 1.00 | 28.45 | C |
| ATOM | 879 | CG | LYS A 124 | 14.153 | 7.783 | 43.204 | 1.00 | 29.42 | C |
| ATOM | 880 | CD | LYS A 124 | 15.597 | 7.442 | 42.804 | 1.00 | 30.46 | C |
| ATOM | 881 | CE | LYS A 124 | 16.479 | 7.067 | 43.992 | 1.00 | 30.52 | C |
| ATOM | 882 | NZ | LYS A 124 | 17.928 | 7.324 | 43.699 | 1.00 | 30.05 | N |
| ATOM | 883 | N | PHE A 125 | 13.188 | 9.407 | 39.014 | 1.00 | 26.98 | N |
| ATOM | 884 | CA | PHE A 125 | 12.477 | 9.871 | 37.826 | 1.00 | 26.83 | C |
| ATOM | 885 | C | PHE A 125 | 10.974 | 9.762 | 37.972 | 1.00 | 26.77 | C |
| ATOM | 886 | O | PHE A 125 | 10.245 | 10.673 | 37.585 | 1.00 | 26.38 | O |
| ATOM | 887 | CB | PHE A 125 | 12.927 | 9.138 | 36.568 | 1.00 | 26.71 | C |
| ATOM | 888 | CG | PHE A 125 | 12.613 | 9.891 | 35.316 | 1.00 | 26.32 | C |
| ATOM | 889 | CD1 | PHE A 125 | 13.476 | 10.876 | 34.849 | 1.00 | 26.29 | C |
| ATOM | 890 | CD2 | PHE A 125 | 11.438 | 9.657 | 34.635 | 1.00 | 26.06 | C |
| ATOM | 891 | CE1 | PHE A 125 | 13.183 | 11.594 | 33.715 | 1.00 | 25.70 | C |
| ATOM | 892 | CE2 | PHE A 125 | 11.140 | 10.368 | 33.483 | 1.00 | 26.70 | C |
| ATOM | 893 | CZ | PHE A 125 | 12.018 | 11.341 | 33.025 | 1.00 | 26.87 | C |
| ATOM | 894 | N | HIS A 126 | 10.527 | 8.649 | 38.550 | 1.00 | 26.77 | N |
| ATOM | 895 | CA | HIS A 126 | 9.113 | 8.396 | 38.753 | 1.00 | 26.82 | C |
| ATOM | 896 | C | HIS A 126 | 8.517 | 9.390 | 39.734 | 1.00 | 26.68 | C |
| ATOM | 897 | O | HIS A 126 | 7.326 | 9.670 | 39.687 | 1.00 | 26.03 | O |
| ATOM | 898 | CB | HIS A 126 | 8.882 | 6.951 | 39.238 | 1.00 | 27.07 | C |
| ATOM | 899 | CG | HIS A 126 | 9.028 | 6.767 | 40.717 | 1.00 | 27.39 | C |
| ATOM | 900 | ND1 | HIS A 126 | 7.959 | 6.836 | 41.582 | 1.00 | 28.48 | N |
| ATOM | 901 | CD2 | HIS A 126 | 10.115 | 6.505 | 41.484 | 1.00 | 28.33 | C |
| ATOM | 902 | CE1 | HIS A 126 | 8.382 | 6.636 | 42.819 | 1.00 | 28.68 | C |
| ATOM | 903 | NE2 | HIS A 126 | 9.687 | 6.439 | 42.788 | 1.00 | 27.97 | N |
| ATOM | 904 | N | GLU A 127 | 9.342 | 9.918 | 40.630 | 1.00 | 27.00 | N |
| ATOM | 905 | CA | GLU A 127 | 8.876 | 10.930 | 41.572 | 1.00 | 27.34 | C |
| ATOM | 906 | C | GLU A 127 | 8.683 | 12.259 | 40.838 | 1.00 | 27.36 | C |
| ATOM | 907 | O | GLU A 127 | 7.761 | 13.026 | 41.126 | 1.00 | 26.86 | O |
| ATOM | 908 | CB | GLU A 127 | 9.862 | 11.084 | 42.728 | 1.00 | 27.31 | C |
| ATOM | 909 | CG | GLU A 127 | 10.018 | 9.821 | 43.552 | 1.00 | 28.69 | C |
| ATOM | 910 | CD | GLU A 127 | 10.959 | 9.992 | 44.722 | 1.00 | 29.65 | C |
| ATOM | 911 | OE1 | GLU A 127 | 12.139 | 10.318 | 44.485 | 1.00 | 29.56 | O |
| ATOM | 912 | OE2 | GLU A 127 | 10.509 | 9.787 | 45.876 | 1.00 | 30.92 | O |
| ATOM | 913 | N | PHE A 128 | 9.554 | 12.519 | 39.876 | 1.00 | 27.91 | N |
| ATOM | 914 | CA | PHE A 128 | 9.453 | 13.736 | 39.068 | 1.00 | 28.21 | C |
| ATOM | 915 | C | PHE A 128 | 8.149 | 13.658 | 38.282 | 1.00 | 29.04 | C |
| ATOM | 916 | O | PHE A 128 | 7.354 | 14.600 | 38.255 | 1.00 | 29.03 | O |
| ATOM | 917 | CB | PHE A 128 | 10.643 | 13.838 | 38.115 | 1.00 | 27.74 | C |
| ATOM | 918 | CG | PHE A 128 | 10.427 | 14.792 | 36.959 | 1.00 | 27.06 | C |
| ATOM | 919 | CD1 | PHE A 128 | 10.189 | 16.138 | 37.185 | 1.00 | 25.41 | C |
| ATOM | 920 | CD2 | PHE A 128 | 10.480 | 14.343 | 35.657 | 1.00 | 25.60 | C |
| ATOM | 921 | CE1 | PHE A 128 | 9.985 | 17.000 | 36.144 | 1.00 | 25.41 | C |
| ATOM | 922 | CE2 | PHE A 128 | 10.281 | 15.215 | 34.604 | 1.00 | 26.59 | C |
| ATOM | 923 | CZ | PHE A 128 | 10.032 | 16.540 | 34.846 | 1.00 | 25.61 | C |
| ATOM | 924 | N | VAL A 129 | 7.925 | 12.500 | 37.677 | 1.00 | 29.90 | N |
| ATOM | 925 | CA | VAL A 129 | 6.756 | 12.285 | 36.847 | 1.00 | 30.82 | C |
| ATOM | 926 | C | VAL A 129 | 5.476 | 12.447 | 37.669 | 1.00 | 31.61 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 927 | O | VAL | A | 129 | 4.515 | 13.091 | 37.234 | 1.00 | 31.39 | O |
| ATOM | 928 | CB | VAL | A | 129 | 6.793 | 10.883 | 36.213 | 1.00 | 30.92 | C |
| ATOM | 929 | CG1 | VAL | A | 129 | 5.479 | 10.582 | 35.503 | 1.00 | 31.15 | C |
| ATOM | 930 | CG2 | VAL | A | 129 | 7.975 | 10.751 | 35.253 | 1.00 | 30.61 | C |
| ATOM | 931 | N | GLU | A | 130 | 5.475 | 11.858 | 38.861 | 1.00 | 32.42 | N |
| ATOM | 932 | CA | GLU | A | 130 | 4.332 | 11.946 | 39.761 | 1.00 | 33.13 | C |
| ATOM | 933 | C | GLU | A | 130 | 4.070 | 13.403 | 40.126 | 1.00 | 33.42 | C |
| ATOM | 934 | O | GLU | A | 130 | 2.930 | 13.867 | 40.081 | 1.00 | 33.01 | O |
| ATOM | 935 | CB | GLU | A | 130 | 4.587 | 11.108 | 41.017 | 1.00 | 33.20 | C |
| ATOM | 936 | CG | GLU | A | 130 | 4.537 | 9.609 | 40.755 | 1.00 | 34.22 | C |
| ATOM | 937 | CD | GLU | A | 130 | 5.294 | 8.792 | 41.789 | 1.00 | 35.55 | C |
| ATOM | 938 | OE1 | GLU | A | 130 | 5.630 | 9.339 | 42.861 | 1.00 | 37.02 | O |
| ATOM | 939 | OE2 | GLU | A | 130 | 5.558 | 7.598 | 41.525 | 1.00 | 35.99 | O |
| ATOM | 940 | N | LYS | A | 131 | 5.128 | 14.120 | 40.486 | 1.00 | 34.00 | N |
| ATOM | 941 | CA | LYS | A | 131 | 4.994 | 15.538 | 40.800 | 1.00 | 34.79 | C |
| ATOM | 942 | C | LYS | A | 131 | 4.354 | 16.286 | 39.637 | 1.00 | 35.25 | C |
| ATOM | 943 | O | LYS | A | 131 | 3.449 | 17.089 | 39.835 | 1.00 | 34.81 | O |
| ATOM | 944 | CB | LYS | A | 131 | 6.345 | 16.171 | 41.100 | 1.00 | 34.89 | C |
| ATOM | 945 | CG | LYS | A | 131 | 6.597 | 16.477 | 42.554 | 1.00 | 35.57 | C |
| ATOM | 946 | CD | LYS | A | 131 | 7.191 | 17.868 | 42.694 | 1.00 | 36.25 | C |
| ATOM | 947 | CE | LYS | A | 131 | 7.862 | 18.072 | 44.034 | 1.00 | 37.30 | C |
| ATOM | 948 | NZ | LYS | A | 131 | 8.108 | 19.526 | 44.332 | 1.00 | 37.49 | N |
| ATOM | 949 | N | LEU | A | 132 | 4.829 | 16.038 | 38.422 | 1.00 | 36.00 | N |
| ATOM | 950 | CA | LEU | A | 132 | 4.243 | 16.701 | 37.268 | 1.00 | 37.05 | C |
| ATOM | 951 | C | LEU | A | 132 | 2.755 | 16.406 | 37.170 | 1.00 | 37.67 | C |
| ATOM | 952 | O | LEU | A | 132 | 1.963 | 17.300 | 36.870 | 1.00 | 37.77 | O |
| ATOM | 953 | CB | LEU | A | 132 | 4.919 | 16.260 | 35.979 | 1.00 | 37.39 | C |
| ATOM | 954 | CG | LEU | A | 132 | 6.310 | 16.803 | 35.710 | 1.00 | 38.29 | C |
| ATOM | 955 | CD1 | LEU | A | 132 | 6.783 | 16.289 | 34.363 | 1.00 | 39.35 | C |
| ATOM | 956 | CD2 | LEU | A | 132 | 6.306 | 18.314 | 35.721 | 1.00 | 39.70 | C |
| ATOM | 957 | N | GLN | A | 133 | 2.386 | 15.151 | 37.417 | 1.00 | 38.34 | N |
| ATOM | 958 | CA | GLN | A | 133 | 0.989 | 14.730 | 37.373 | 1.00 | 39.11 | C |
| ATOM | 959 | C | GLN | A | 133 | 0.132 | 15.434 | 38.427 | 1.00 | 39.73 | C |
| ATOM | 960 | O | GLN | A | 133 | -0.966 | 15.897 | 38.126 | 1.00 | 39.61 | O |
| ATOM | 961 | CB | GLN | A | 133 | 0.886 | 13.213 | 37.538 | 1.00 | 39.05 | C |
| ATOM | 962 | N | ASP | A | 134 | 0.629 | 15.507 | 39.658 | 1.00 | 40.61 | N |
| ATOM | 963 | CA | ASP | A | 134 | -0.108 | 16.149 | 40.747 | 1.00 | 41.70 | C |
| ATOM | 964 | C | ASP | A | 134 | -0.398 | 17.626 | 40.451 | 1.00 | 41.68 | C |
| ATOM | 965 | O | ASP | A | 134 | -1.470 | 18.137 | 40.770 | 1.00 | 41.28 | O |
| ATOM | 966 | CB | ASP | A | 134 | 0.678 | 16.030 | 42.056 | 1.00 | 42.32 | C |
| ATOM | 967 | CG | ASP | A | 134 | -0.165 | 16.351 | 43.286 | 1.00 | 44.92 | C |
| ATOM | 968 | OD1 | ASP | A | 134 | -1.235 | 16.991 | 43.152 | 1.00 | 48.33 | O |
| ATOM | 969 | OD2 | ASP | A | 134 | 0.164 | 15.991 | 44.442 | 1.00 | 48.64 | O |
| ATOM | 970 | N | ILE | A | 135 | 0.563 | 18.312 | 39.842 | 1.00 | 41.92 | N |
| ATOM | 971 | CA | ILE | A | 135 | 0.383 | 19.717 | 39.512 | 1.00 | 42.18 | C |
| ATOM | 972 | C | ILE | A | 135 | -0.715 | 19.862 | 38.471 | 1.00 | 42.41 | C |
| ATOM | 973 | O | ILE | A | 135 | -1.635 | 20.664 | 38.634 | 1.00 | 42.49 | O |
| ATOM | 974 | CB | ILE | A | 135 | 1.696 | 20.324 | 38.997 | 1.00 | 42.17 | C |
| ATOM | 975 | CG1 | ILE | A | 135 | 2.720 | 20.399 | 40.131 | 1.00 | 42.25 | C |
| ATOM | 976 | CG2 | ILE | A | 135 | 1.451 | 21.708 | 38.437 | 1.00 | 42.11 | C |
| ATOM | 977 | CD1 | ILE | A | 135 | 4.151 | 20.438 | 39.653 | 1.00 | 42.91 | C |
| ATOM | 978 | N | GLN | A | 136 | -0.614 | 19.075 | 37.407 | 1.00 | 42.71 | N |
| ATOM | 979 | CA | GLN | A | 136 | -1.593 | 19.114 | 36.333 | 1.00 | 43.09 | C |
| ATOM | 980 | C | GLN | A | 136 | -2.991 | 18.935 | 36.900 | 1.00 | 43.56 | C |
| ATOM | 981 | O | GLN | A | 136 | -3.863 | 19.785 | 36.707 | 1.00 | 43.93 | O |
| ATOM | 982 | CB | GLN | A | 136 | -1.298 | 18.031 | 35.317 | 1.00 | 43.10 | C |
| ATOM | 983 | N | GLN | A | 137 | -3.181 | 17.844 | 37.635 | 1.00 | 43.82 | N |
| ATOM | 984 | CA | GLN | A | 137 | -4.486 | 17.493 | 38.182 | 1.00 | 44.02 | C |
| ATOM | 985 | C | GLN | A | 137 | -5.023 | 18.540 | 39.144 | 1.00 | 44.08 | C |
| ATOM | 986 | O | GLN | A | 137 | -6.202 | 18.891 | 39.080 | 1.00 | 44.46 | O |
| ATOM | 987 | CB | GLN | A | 137 | -4.425 | 16.124 | 38.868 | 1.00 | 44.00 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 988 | N | ARG | A | 138 | -4.169 | 19.043 | 40.031 | 1.00 43.93 | N |
| ATOM | 989 | CA | ARG | A | 138 | -4.606 | 20.022 | 41.024 | 1.00 43.76 | C |
| ATOM | 990 | C | ARG | A | 138 | -4.578 | 21.445 | 40.463 | 1.00 43.34 | C |
| ATOM | 991 | O | ARG | A | 138 | -4.681 | 22.415 | 41.214 | 1.00 43.54 | O |
| ATOM | 992 | CB | ARG | A | 138 | -3.751 | 19.919 | 42.299 | 1.00 43.84 | C |
| ATOM | 993 | CG | ARG | A | 138 | -2.420 | 20.679 | 42.279 | 1.00 44.85 | C |
| ATOM | 994 | CD | ARG | A | 138 | -1.493 | 20.279 | 43.420 | 1.00 45.82 | C |
| ATOM | 995 | NE | ARG | A | 138 | -0.372 | 21.197 | 43.620 | 1.00 46.44 | N |
| ATOM | 996 | CZ | ARG | A | 138 | 0.914 | 20.863 | 43.499 | 1.00 47.95 | C |
| ATOM | 997 | NH1 | ARG | A | 138 | 1.262 | 19.627 | 43.162 | 1.00 49.02 | N |
| ATOM | 998 | NH2 | ARG | A | 138 | 1.864 | 21.767 | 43.709 | 1.00 47.70 | N |
| ATOM | 999 | N | GLY | A | 139 | -4.450 | 21.569 | 39.143 | 1.00 42.62 | N |
| ATOM | 1000 | CA | GLY | A | 139 | -4.371 | 22.871 | 38.504 | 1.00 41.93 | C |
| ATOM | 1001 | C | GLY | A | 139 | -3.389 | 23.820 | 39.174 | 1.00 41.28 | C |
| ATOM | 1002 | O | GLY | A | 139 | -3.607 | 25.030 | 39.196 | 1.00 41.58 | O |
| ATOM | 1003 | N | GLY | A | 140 | -2.291 | 23.292 | 39.703 | 1.00 40.31 | N |
| ATOM | 1004 | CA | GLY | A | 140 | -1.329 | 24.119 | 40.410 | 1.00 39.43 | C |
| ATOM | 1005 | C | GLY | A | 140 | -0.563 | 25.070 | 39.512 | 1.00 38.71 | C |
| ATOM | 1006 | O | GLY | A | 140 | -0.495 | 24.871 | 38.294 | 1.00 38.40 | O |
| ATOM | 1007 | N | GLU | A | 141 | 0.003 | 26.117 | 40.110 | 1.00 37.82 | N |
| ATOM | 1008 | CA | GLU | A | 141 | 0.829 | 27.066 | 39.363 | 1.00 37.20 | C |
| ATOM | 1009 | C | GLU | A | 141 | 2.320 | 26.726 | 39.491 | 1.00 35.94 | C |
| ATOM | 1010 | O | GLU | A | 141 | 3.160 | 27.356 | 38.845 | 1.00 35.76 | O |
| ATOM | 1011 | CB | GLU | A | 141 | 0.590 | 28.510 | 39.828 | 1.00 37.63 | C |
| ATOM | 1012 | CG | GLU | A | 141 | -0.729 | 29.146 | 39.379 | 1.00 39.51 | C |
| ATOM | 1013 | CD | GLU | A | 141 | -0.936 | 29.164 | 37.866 | 1.00 41.63 | C |
| ATOM | 1014 | OE1 | GLU | A | 141 | 0.056 | 29.147 | 37.102 | 1.00 42.42 | O |
| ATOM | 1015 | OE2 | GLU | A | 141 | -2.115 | 29.202 | 37.434 | 1.00 43.77 | O |
| ATOM | 1016 | N | GLU | A | 142 | 2.652 | 25.742 | 40.326 | 1.00 34.29 | N |
| ATOM | 1017 | CA | GLU | A | 142 | 4.045 | 25.351 | 40.510 | 1.00 33.08 | C |
| ATOM | 1018 | C | GLU | A | 142 | 4.655 | 24.938 | 39.170 | 1.00 31.87 | C |
| ATOM | 1019 | O | GLU | A | 142 | 3.958 | 24.443 | 38.296 | 1.00 31.87 | O |
| ATOM | 1020 | CB | GLU | A | 142 | 4.170 | 24.201 | 41.519 | 1.00 32.96 | C |
| ATOM | 1021 | CG | GLU | A | 142 | 5.610 | 23.914 | 41.942 | 1.00 32.71 | C |
| ATOM | 1022 | CD | GLU | A | 142 | 5.761 | 22.730 | 42.896 | 1.00 33.55 | C |
| ATOM | 1023 | OE1 | GLU | A | 142 | 4.778 | 22.001 | 43.146 | 1.00 32.41 | O |
| ATOM | 1024 | OE2 | GLU | A | 142 | 6.888 | 22.520 | 43.398 | 1.00 34.13 | O |
| ATOM | 1025 | N | ARG | A | 143 | 5.954 | 25.156 | 39.017 | 1.00 30.56 | N |
| ATOM | 1026 | CA | ARG | A | 143 | 6.662 | 24.766 | 37.803 | 1.00 29.79 | C |
| ATOM | 1027 | C | ARG | A | 143 | 7.878 | 23.939 | 38.142 | 1.00 28.70 | C |
| ATOM | 1028 | O | ARG | A | 143 | 8.565 | 24.210 | 39.127 | 1.00 28.88 | O |
| ATOM | 1029 | CB | ARG | A | 143 | 7.142 | 25.991 | 37.040 | 1.00 29.90 | C |
| ATOM | 1030 | CG | ARG | A | 143 | 6.043 | 26.832 | 36.441 | 1.00 30.80 | C |
| ATOM | 1031 | CD | ARG | A | 143 | 6.591 | 27.992 | 35.636 | 1.00 30.70 | C |
| ATOM | 1032 | NE | ARG | A | 143 | 5.538 | 28.715 | 34.935 | 1.00 30.86 | N |
| ATOM | 1033 | CZ | ARG | A | 143 | 5.168 | 28.487 | 33.682 | 1.00 29.53 | C |
| ATOM | 1034 | NH1 | ARG | A | 143 | 5.763 | 27.547 | 32.941 | 1.00 27.51 | N |
| ATOM | 1035 | NH2 | ARG | A | 143 | 4.196 | 29.216 | 33.168 | 1.00 30.04 | N |
| ATOM | 1036 | N | LEU | A | 144 | 8.156 | 22.943 | 37.315 | 1.00 27.27 | N |
| ATOM | 1037 | CA | LEU | A | 144 | 9.319 | 22.102 | 37.518 | 1.00 26.47 | C |
| ATOM | 1038 | C | LEU | A | 144 | 10.220 | 22.148 | 36.297 | 1.00 25.40 | C |
| ATOM | 1039 | O | LEU | A | 144 | 9.755 | 22.330 | 35.172 | 1.00 25.39 | O |
| ATOM | 1040 | CB | LEU | A | 144 | 8.893 | 20.652 | 37.753 | 1.00 26.70 | C |
| ATOM | 1041 | CG | LEU | A | 144 | 7.922 | 20.416 | 38.915 | 1.00 27.15 | C |
| ATOM | 1042 | CD1 | LEU | A | 144 | 7.575 | 18.921 | 39.059 | 1.00 27.40 | C |
| ATOM | 1043 | CD2 | LEU | A | 144 | 8.488 | 20.956 | 40.221 | 1.00 27.42 | C |
| ATOM | 1044 | N | TYR | A | 145 | 11.511 | 21.974 | 36.527 | 1.00 23.90 | N |
| ATOM | 1045 | CA | TYR | A | 145 | 12.458 | 21.871 | 35.441 | 1.00 23.15 | C |
| ATOM | 1046 | C | TYR | A | 145 | 13.516 | 20.857 | 35.868 | 1.00 23.04 | C |
| ATOM | 1047 | O | TYR | A | 145 | 14.328 | 21.130 | 36.740 | 1.00 22.58 | O |
| ATOM | 1048 | CB | TYR | A | 145 | 13.080 | 23.235 | 35.107 | 1.00 23.01 | C |

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ATOM   1049  CG  TYR A 145      13.522  23.419  33.666  1.00 21.34           C
ATOM   1050  CD1 TYR A 145      13.824  22.333  32.863  1.00 20.11           C
ATOM   1051  CD2 TYR A 145      13.662  24.691  33.119  1.00 21.14           C
ATOM   1052  CE1 TYR A 145      14.219  22.494  31.563  1.00 20.22           C
ATOM   1053  CE2 TYR A 145      14.075  24.866  31.807  1.00 19.81           C
ATOM   1054  CZ  TYR A 145      14.349  23.764  31.027  1.00 19.19           C
ATOM   1055  OH  TYR A 145      14.736  23.903  29.699  1.00 18.36           O
ATOM   1056  N   LEU A 146      13.461  19.666  35.287  1.00 22.75           N
ATOM   1057  CA  LEU A 146      14.490  18.661  35.516  1.00 23.17           C
ATOM   1058  C   LEU A 146      15.720  19.005  34.679  1.00 22.99           C
ATOM   1059  O   LEU A 146      15.604  19.264  33.490  1.00 22.81           O
ATOM   1060  CB  LEU A 146      13.980  17.282  35.115  1.00 23.33           C
ATOM   1061  CG  LEU A 146      14.992  16.141  35.274  1.00 24.98           C
ATOM   1062  CD1 LEU A 146      14.276  14.846  35.622  1.00 24.56           C
ATOM   1063  CD2 LEU A 146      15.849  15.946  34.016  1.00 26.13           C
ATOM   1064  N   GLN A 147      16.891  18.983  35.299  1.00 23.05           N
ATOM   1065  CA  GLN A 147      18.135  19.314  34.619  1.00 23.65           C
ATOM   1066  C   GLN A 147      19.158  18.394  35.231  1.00 23.86           C
ATOM   1067  O   GLN A 147      19.573  18.597  36.364  1.00 24.61           O
ATOM   1068  CB  GLN A 147      18.516  20.793  34.821  1.00 23.53           C
ATOM   1069  CG  GLN A 147      17.386  21.770  34.461  1.00 24.34           C
ATOM   1070  CD  GLN A 147      17.800  23.238  34.482  1.00 26.20           C
ATOM   1071  OE1 GLN A 147      17.034  24.114  34.035  1.00 29.67           O
ATOM   1072  NE2 GLN A 147      18.979  23.514  34.988  1.00 21.33           N
ATOM   1073  N   GLN A 148      19.542  17.369  34.485  1.00 24.35           N
ATOM   1074  CA  GLN A 148      20.393  16.314  35.006  1.00 24.70           C
ATOM   1075  C   GLN A 148      21.319  15.753  33.964  1.00 25.16           C
ATOM   1076  O   GLN A 148      20.898  15.378  32.866  1.00 24.21           O
ATOM   1077  CB  GLN A 148      19.525  15.172  35.526  1.00 24.97           C
ATOM   1078  CG  GLN A 148      20.317  13.940  35.953  1.00 25.54           C
ATOM   1079  CD  GLN A 148      21.275  14.256  37.085  1.00 26.98           C
ATOM   1080  OE1 GLN A 148      20.892  14.941  38.042  1.00 26.73           O
ATOM   1081  NE2 GLN A 148      22.522  13.786  36.976  1.00 26.37           N
ATOM   1082  N   THR A 149      22.592  15.704  34.321  1.00 25.94           N
ATOM   1083  CA  THR A 149      23.603  15.134  33.466  1.00 27.43           C
ATOM   1084  C   THR A 149      23.369  13.632  33.324  1.00 27.29           C
ATOM   1085  O   THR A 149      23.081  12.965  34.303  1.00 27.40           O
ATOM   1086  CB  THR A 149      24.990  15.430  34.075  1.00 27.91           C
ATOM   1087  OG1 THR A 149      25.282  16.829  33.901  1.00 30.41           O
ATOM   1088  CG2 THR A 149      26.078  14.776  33.276  1.00 30.12           C
ATOM   1089  N   LEU A 150      23.461  13.117  32.100  1.00 27.79           N
ATOM   1090  CA  LEU A 150      23.321  11.690  31.832  1.00 28.02           C
ATOM   1091  C   LEU A 150      24.549  10.935  32.364  1.00 28.42           C
ATOM   1092  O   LEU A 150      25.682  11.261  32.002  1.00 28.86           O
ATOM   1093  CB  LEU A 150      23.194  11.435  30.326  1.00 28.08           C
ATOM   1094  CG  LEU A 150      21.929  11.937  29.622  1.00 28.70           C
ATOM   1095  CD1 LEU A 150      22.016  11.725  28.117  1.00 28.62           C
ATOM   1096  CD2 LEU A 150      20.697  11.260  30.175  1.00 29.47           C
ATOM   1097  N   ASN A 151      24.332   9.928  33.203  1.00 28.58           N
ATOM   1098  CA  ASN A 151      25.434   9.156  33.781  1.00 28.79           C
ATOM   1099  C   ASN A 151      25.194   7.636  33.782  1.00 29.24           C
ATOM   1100  O   ASN A 151      24.197   7.163  33.238  1.00 29.60           O
ATOM   1101  CB  ASN A 151      25.657   9.631  35.208  1.00 28.77           C
ATOM   1102  CG  ASN A 151      24.459   9.367  36.084  1.00 28.05           C
ATOM   1103  OD1 ASN A 151      23.936   8.246  36.126  1.00 29.02           O
ATOM   1104  ND2 ASN A 151      24.000  10.396  36.772  1.00 26.99           N
ATOM   1105  N   ASP A 152      26.083   6.885  34.437  1.00 29.71           N
ATOM   1106  CA  ASP A 152      26.039   5.410  34.448  1.00 30.06           C
ATOM   1107  C   ASP A 152      24.850   4.733  35.075  1.00 29.51           C
ATOM   1108  O   ASP A 152      24.771   3.503  35.026  1.00 28.98           O
ATOM   1109  CB  ASP A 152      27.199   4.829  35.250  1.00 30.99           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1110 | CG | ASP | A | 152 | 28.447 | 5.561 | 35.048 | 1.00 | 33.80 | C |
| ATOM | 1111 | OD1 | ASP | A | 152 | 28.636 | 6.071 | 33.918 | 1.00 | 40.13 | O |
| ATOM | 1112 | OD2 | ASP | A | 152 | 29.274 | 5.719 | 35.960 | 1.00 | 35.65 | O |
| ATOM | 1113 | N | THR | A | 153 | 23.959 | 5.468 | 35.722 | 1.00 | 28.96 | N |
| ATOM | 1114 | CA | THR | A | 153 | 22.831 | 4.792 | 36.359 | 1.00 | 28.42 | C |
| ATOM | 1115 | C | THR | A | 153 | 21.685 | 4.594 | 35.387 | 1.00 | 27.75 | C |
| ATOM | 1116 | O | THR | A | 153 | 20.730 | 3.909 | 35.712 | 1.00 | 27.68 | O |
| ATOM | 1117 | CB | THR | A | 153 | 22.330 | 5.552 | 37.584 | 1.00 | 28.53 | C |
| ATOM | 1118 | OG1 | THR | A | 153 | 21.833 | 6.836 | 37.193 | 1.00 | 28.91 | O |
| ATOM | 1119 | CG2 | THR | A | 153 | 23.473 | 5.855 | 38.540 | 1.00 | 29.18 | C |
| ATOM | 1120 | N | VAL | A | 154 | 21.766 | 5.171 | 34.194 | 1.00 | 26.76 | N |
| ATOM | 1121 | CA | VAL | A | 154 | 20.671 | 4.996 | 33.246 | 1.00 | 26.61 | C |
| ATOM | 1122 | C | VAL | A | 154 | 20.583 | 3.531 | 32.895 | 1.00 | 26.77 | C |
| ATOM | 1123 | O | VAL | A | 154 | 21.592 | 2.832 | 32.923 | 1.00 | 27.36 | O |
| ATOM | 1124 | CB | VAL | A | 154 | 20.838 | 5.826 | 31.964 | 1.00 | 26.05 | C |
| ATOM | 1125 | CG1 | VAL | A | 154 | 20.914 | 7.279 | 32.312 | 1.00 | 26.14 | C |
| ATOM | 1126 | CG2 | VAL | A | 154 | 22.071 | 5.383 | 31.182 | 1.00 | 25.62 | C |
| ATOM | 1127 | N | GLY | A | 155 | 19.379 | 3.072 | 32.568 | 1.00 | 26.71 | N |
| ATOM | 1128 | CA | GLY | A | 155 | 19.147 | 1.674 | 32.252 | 1.00 | 26.42 | C |
| ATOM | 1129 | C | GLY | A | 155 | 19.531 | 1.266 | 30.840 | 1.00 | 26.67 | C |
| ATOM | 1130 | O | GLY | A | 155 | 19.894 | 2.093 | 29.983 | 1.00 | 26.52 | O |
| ATOM | 1131 | N | ARG | A | 156 | 19.390 | -0.028 | 30.599 | 1.00 | 26.49 | N |
| ATOM | 1132 | CA | ARG | A | 156 | 19.811 | -0.684 | 29.364 | 1.00 | 26.54 | C |
| ATOM | 1133 | C | ARG | A | 156 | 19.305 | -0.053 | 28.068 | 1.00 | 25.95 | C |
| ATOM | 1134 | O | ARG | A | 156 | 20.089 | 0.194 | 27.160 | 1.00 | 26.26 | O |
| ATOM | 1135 | CB | ARG | A | 156 | 19.429 | -2.165 | 29.418 | 1.00 | 26.28 | C |
| ATOM | 1136 | N | LYS | A | 157 | 18.004 | 0.175 | 27.964 | 1.00 | 25.43 | N |
| ATOM | 1137 | CA | LYS | A | 157 | 17.460 | 0.777 | 26.756 | 1.00 | 25.11 | C |
| ATOM | 1138 | C | LYS | A | 157 | 18.026 | 2.198 | 26.517 | 1.00 | 25.50 | C |
| ATOM | 1139 | O | LYS | A | 157 | 18.249 | 2.595 | 25.372 | 1.00 | 25.14 | O |
| ATOM | 1140 | CB | LYS | A | 157 | 15.927 | 0.796 | 26.809 | 1.00 | 24.88 | C |
| ATOM | 1141 | CG | LYS | A | 157 | 15.255 | -0.572 | 26.516 | 1.00 | 24.25 | C |
| ATOM | 1142 | N | ILE | A | 158 | 18.257 | 2.956 | 27.585 | 1.00 | 25.35 | N |
| ATOM | 1143 | CA | ILE | A | 158 | 18.766 | 4.326 | 27.432 | 1.00 | 25.61 | C |
| ATOM | 1144 | C | ILE | A | 158 | 20.205 | 4.250 | 26.971 | 1.00 | 25.76 | C |
| ATOM | 1145 | O | ILE | A | 158 | 20.661 | 5.058 | 26.166 | 1.00 | 25.39 | O |
| ATOM | 1146 | CB | ILE | A | 158 | 18.662 | 5.107 | 28.740 | 1.00 | 25.41 | C |
| ATOM | 1147 | CG1 | ILE | A | 158 | 17.202 | 5.245 | 29.162 | 1.00 | 25.92 | C |
| ATOM | 1148 | CG2 | ILE | A | 158 | 19.297 | 6.475 | 28.601 | 1.00 | 25.61 | C |
| ATOM | 1149 | CD1 | ILE | A | 158 | 16.331 | 5.924 | 28.174 | 1.00 | 27.88 | C |
| ATOM | 1150 | N | VAL | A | 159 | 20.909 | 3.251 | 27.481 | 1.00 | 26.10 | N |
| ATOM | 1151 | CA | VAL | A | 159 | 22.276 | 3.010 | 27.079 | 1.00 | 26.57 | C |
| ATOM | 1152 | C | VAL | A | 159 | 22.279 | 2.703 | 25.585 | 1.00 | 26.40 | C |
| ATOM | 1153 | O | VAL | A | 159 | 23.074 | 3.248 | 24.840 | 1.00 | 26.32 | O |
| ATOM | 1154 | CB | VAL | A | 159 | 22.895 | 1.850 | 27.883 | 1.00 | 26.94 | C |
| ATOM | 1155 | CG1 | VAL | A | 159 | 24.136 | 1.310 | 27.193 | 1.00 | 27.73 | C |
| ATOM | 1156 | CG2 | VAL | A | 159 | 23.223 | 2.308 | 29.298 | 1.00 | 26.73 | C |
| ATOM | 1157 | N | MET | A | 160 | 21.363 | 1.852 | 25.145 | 1.00 | 26.48 | N |
| ATOM | 1158 | CA | MET | A | 160 | 21.270 | 1.518 | 23.721 | 1.00 | 26.52 | C |
| ATOM | 1159 | C | MET | A | 160 | 20.985 | 2.771 | 22.880 | 1.00 | 25.02 | C |
| ATOM | 1160 | O | MET | A | 160 | 21.600 | 2.986 | 21.845 | 1.00 | 24.31 | O |
| ATOM | 1161 | CB | MET | A | 160 | 20.183 | 0.476 | 23.485 | 1.00 | 27.05 | C |
| ATOM | 1162 | CG | MET | A | 160 | 20.540 | -0.900 | 24.001 | 1.00 | 30.45 | C |
| ATOM | 1163 | SD | MET | A | 160 | 21.843 | -1.730 | 23.058 | 1.00 | 34.87 | S |
| ATOM | 1164 | CE | MET | A | 160 | 20.957 | -2.028 | 21.496 | 1.00 | 36.94 | C |
| ATOM | 1165 | N | ASP | A | 161 | 20.047 | 3.589 | 23.342 | 1.00 | 23.96 | N |
| ATOM | 1166 | CA | ASP | A | 161 | 19.699 | 4.831 | 22.665 | 1.00 | 23.14 | C |
| ATOM | 1167 | C | ASP | A | 161 | 20.890 | 5.781 | 22.550 | 1.00 | 21.93 | C |
| ATOM | 1168 | O | ASP | A | 161 | 21.167 | 6.323 | 21.480 | 1.00 | 21.41 | O |
| ATOM | 1169 | CB | ASP | A | 161 | 18.549 | 5.528 | 23.402 | 1.00 | 23.13 | C |
| ATOM | 1170 | CG | ASP | A | 161 | 17.250 | 4.762 | 23.293 | 1.00 | 24.08 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1171 | OD1 | ASP | A | 161 | 17.182 | 3.812 | 22.478 | 1.00 | 21.27 | O |
| ATOM | 1172 | OD2 | ASP | A | 161 | 16.248 | 5.035 | 23.980 | 1.00 | 25.87 | O |
| ATOM | 1173 | N | PHE | A | 162 | 21.575 | 5.973 | 23.671 | 1.00 | 20.59 | N |
| ATOM | 1174 | CA | PHE | A | 162 | 22.712 | 6.859 | 23.765 | 1.00 | 19.97 | C |
| ATOM | 1175 | C | PHE | A | 162 | 23.802 | 6.409 | 22.809 | 1.00 | 19.19 | C |
| ATOM | 1176 | O | PHE | A | 162 | 24.410 | 7.213 | 22.160 | 1.00 | 18.98 | O |
| ATOM | 1177 | CB | PHE | A | 162 | 23.223 | 6.859 | 25.220 | 1.00 | 20.44 | C |
| ATOM | 1178 | CG | PHE | A | 162 | 24.386 | 7.755 | 25.470 | 1.00 | 20.78 | C |
| ATOM | 1179 | CD1 | PHE | A | 162 | 24.206 | 9.107 | 25.673 | 1.00 | 25.50 | C |
| ATOM | 1180 | CD2 | PHE | A | 162 | 25.662 | 7.245 | 25.542 | 1.00 | 23.71 | C |
| ATOM | 1181 | CE1 | PHE | A | 162 | 25.290 | 9.930 | 25.935 | 1.00 | 25.85 | C |
| ATOM | 1182 | CE2 | PHE | A | 162 | 26.755 | 8.072 | 25.795 | 1.00 | 24.89 | C |
| ATOM | 1183 | CZ | PHE | A | 162 | 26.572 | 9.394 | 26.001 | 1.00 | 23.50 | C |
| ATOM | 1184 | N | LEU | A | 163 | 24.062 | 5.115 | 22.744 | 1.00 | 19.25 | N |
| ATOM | 1185 | CA | LEU | A | 163 | 25.084 | 4.597 | 21.838 | 1.00 | 19.42 | C |
| ATOM | 1186 | C | LEU | A | 163 | 24.715 | 4.804 | 20.361 | 1.00 | 18.63 | C |
| ATOM | 1187 | O | LEU | A | 163 | 25.585 | 4.831 | 19.493 | 1.00 | 18.21 | O |
| ATOM | 1188 | CB | LEU | A | 163 | 25.297 | 3.115 | 22.104 | 1.00 | 19.49 | C |
| ATOM | 1189 | CG | LEU | A | 163 | 25.988 | 2.812 | 23.422 | 1.00 | 20.88 | C |
| ATOM | 1190 | CD1 | LEU | A | 163 | 25.980 | 1.319 | 23.651 | 1.00 | 22.44 | C |
| ATOM | 1191 | CD2 | LEU | A | 163 | 27.407 | 3.368 | 23.396 | 1.00 | 21.73 | C |
| ATOM | 1192 | N | GLY | A | 164 | 23.419 | 4.917 | 20.104 | 1.00 | 18.01 | N |
| ATOM | 1193 | CA | GLY | A | 164 | 22.889 | 5.158 | 18.779 | 1.00 | 18.55 | C |
| ATOM | 1194 | C | GLY | A | 164 | 22.873 | 6.622 | 18.355 | 1.00 | 18.40 | C |
| ATOM | 1195 | O | GLY | A | 164 | 22.406 | 6.921 | 17.256 | 1.00 | 19.24 | O |
| ATOM | 1196 | N | PHE | A | 165 | 23.365 | 7.521 | 19.209 | 1.00 | 17.50 | N |
| ATOM | 1197 | CA | PHE | A | 165 | 23.493 | 8.913 | 18.831 | 1.00 | 17.67 | C |
| ATOM | 1198 | C | PHE | A | 165 | 24.497 | 8.955 | 17.663 | 1.00 | 17.49 | C |
| ATOM | 1199 | O | PHE | A | 165 | 25.293 | 8.028 | 17.497 | 1.00 | 16.10 | O |
| ATOM | 1200 | CB | PHE | A | 165 | 23.984 | 9.753 | 20.018 | 1.00 | 17.47 | C |
| ATOM | 1201 | CG | PHE | A | 165 | 22.932 | 10.004 | 21.098 | 1.00 | 18.51 | C |
| ATOM | 1202 | CD1 | PHE | A | 165 | 21.645 | 9.479 | 21.009 | 1.00 | 19.26 | C |
| ATOM | 1203 | CD2 | PHE | A | 165 | 23.242 | 10.784 | 22.203 | 1.00 | 18.52 | C |
| ATOM | 1204 | CE1 | PHE | A | 165 | 20.697 | 9.730 | 21.996 | 1.00 | 18.44 | C |
| ATOM | 1205 | CE2 | PHE | A | 165 | 22.303 | 11.030 | 23.199 | 1.00 | 18.52 | C |
| ATOM | 1206 | CZ | PHE | A | 165 | 21.032 | 10.500 | 23.100 | 1.00 | 18.90 | C |
| ATOM | 1207 | N | ASN | A | 166 | 24.466 | 10.009 | 16.854 | 1.00 | 17.77 | N |
| ATOM | 1208 | CA | ASN | A | 166 | 25.393 | 10.110 | 15.712 | 1.00 | 18.29 | C |
| ATOM | 1209 | C | ASN | A | 166 | 26.787 | 10.622 | 16.129 | 1.00 | 18.73 | C |
| ATOM | 1210 | O | ASN | A | 166 | 27.156 | 11.795 | 15.897 | 1.00 | 19.54 | O |
| ATOM | 1211 | CB | ASN | A | 166 | 24.793 | 10.972 | 14.598 | 1.00 | 17.92 | C |
| ATOM | 1212 | CG | ASN | A | 166 | 25.571 | 10.861 | 13.293 | 1.00 | 17.28 | C |
| ATOM | 1213 | OD1 | ASN | A | 166 | 26.679 | 10.289 | 13.262 | 1.00 | 16.53 | O |
| ATOM | 1214 | ND2 | ASN | A | 166 | 24.994 | 11.395 | 12.204 | 1.00 | 12.92 | N |
| ATOM | 1215 | N | TRP | A | 167 | 27.527 | 9.739 | 16.789 | 1.00 | 19.26 | N |
| ATOM | 1216 | CA | TRP | A | 167 | 28.867 | 10.035 | 17.264 | 1.00 | 19.76 | C |
| ATOM | 1217 | C | TRP | A | 167 | 29.785 | 10.266 | 16.084 | 1.00 | 19.88 | C |
| ATOM | 1218 | O | TRP | A | 167 | 30.731 | 11.031 | 16.169 | 1.00 | 19.35 | O |
| ATOM | 1219 | CB | TRP | A | 167 | 29.384 | 8.864 | 18.130 | 1.00 | 19.92 | C |
| ATOM | 1220 | CG | TRP | A | 167 | 28.556 | 8.728 | 19.351 | 1.00 | 20.39 | C |
| ATOM | 1221 | CD1 | TRP | A | 167 | 27.686 | 7.727 | 19.656 | 1.00 | 20.85 | C |
| ATOM | 1222 | CD2 | TRP | A | 167 | 28.445 | 9.686 | 20.400 | 1.00 | 20.99 | C |
| ATOM | 1223 | NE1 | TRP | A | 167 | 27.059 | 7.995 | 20.851 | 1.00 | 21.18 | N |
| ATOM | 1224 | CE2 | TRP | A | 167 | 27.509 | 9.194 | 21.325 | 1.00 | 20.70 | C |
| ATOM | 1225 | CE3 | TRP | A | 167 | 29.065 | 10.916 | 20.664 | 1.00 | 21.55 | C |
| ATOM | 1226 | CZ2 | TRP | A | 167 | 27.183 | 9.871 | 22.488 | 1.00 | 22.63 | C |
| ATOM | 1227 | CZ3 | TRP | A | 167 | 28.731 | 11.589 | 21.804 | 1.00 | 21.78 | C |
| ATOM | 1228 | CH2 | TRP | A | 167 | 27.789 | 11.071 | 22.706 | 1.00 | 22.79 | C |
| ATOM | 1229 | N | ASN | A | 168 | 29.529 | 9.577 | 14.979 | 1.00 | 20.07 | N |
| ATOM | 1230 | CA | ASN | A | 168 | 30.374 | 9.759 | 13.818 | 1.00 | 20.50 | C |
| ATOM | 1231 | C | ASN | A | 168 | 30.396 | 11.237 | 13.421 | 1.00 | 20.67 | C |

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ATOM   1232  O   ASN A 168      31.465  11.806  13.207  1.00 19.54           O
ATOM   1233  CB  ASN A 168      29.917   8.930  12.628  1.00 20.87           C
ATOM   1234  CG  ASN A 168      30.818   9.129  11.423  1.00 22.96           C
ATOM   1235  OD1 ASN A 168      32.027   8.923  11.522  1.00 25.54           O
ATOM   1236  ND2 ASN A 168      30.247   9.578  10.295  1.00 23.09           N
ATOM   1237  N   TRP A 169      29.211  11.844  13.338  1.00 20.57           N
ATOM   1238  CA  TRP A 169      29.106  13.226  12.917  1.00 20.23           C
ATOM   1239  C   TRP A 169      29.653  14.188  13.972  1.00 20.59           C
ATOM   1240  O   TRP A 169      30.367  15.118  13.634  1.00 20.09           O
ATOM   1241  CB  TRP A 169      27.662  13.618  12.570  1.00 20.35           C
ATOM   1242  CG  TRP A 169      27.542  15.101  12.238  1.00 19.49           C
ATOM   1243  CD1 TRP A 169      27.769  15.693  11.026  1.00 19.03           C
ATOM   1244  CD2 TRP A 169      27.203  16.157  13.137  1.00 20.25           C
ATOM   1245  NE1 TRP A 169      27.578  17.052  11.117  1.00 20.36           N
ATOM   1246  CE2 TRP A 169      27.244  17.366  12.406  1.00 19.45           C
ATOM   1247  CE3 TRP A 169      26.874  16.207  14.492  1.00 20.60           C
ATOM   1248  CZ2 TRP A 169      26.964  18.600  12.975  1.00 21.03           C
ATOM   1249  CZ3 TRP A 169      26.614  17.433  15.064  1.00 23.09           C
ATOM   1250  CH2 TRP A 169      26.649  18.621  14.297  1.00 23.61           C
ATOM   1251  N   ILE A 170      29.326  13.979  15.239  1.00 20.47           N
ATOM   1252  CA  ILE A 170      29.759  14.926  16.241  1.00 20.67           C
ATOM   1253  C   ILE A 170      31.262  14.772  16.567  1.00 21.18           C
ATOM   1254  O   ILE A 170      31.943  15.758  16.836  1.00 21.20           O
ATOM   1255  CB  ILE A 170      28.842  14.892  17.483  1.00 20.61           C
ATOM   1256  CG1 ILE A 170      28.900  16.231  18.221  1.00 20.05           C
ATOM   1257  CG2 ILE A 170      29.191  13.755  18.402  1.00 19.89           C
ATOM   1258  CD1 ILE A 170      27.865  16.353  19.329  1.00 21.00           C
ATOM   1259  N   ASN A 171      31.780  13.556  16.527  1.00 20.74           N
ATOM   1260  CA  ASN A 171      33.214  13.355  16.715  1.00 21.80           C
ATOM   1261  C   ASN A 171      34.024  14.093  15.634  1.00 22.34           C
ATOM   1262  O   ASN A 171      35.093  14.652  15.916  1.00 21.98           O
ATOM   1263  CB  ASN A 171      33.581  11.857  16.718  1.00 21.55           C
ATOM   1264  CG  ASN A 171      33.111  11.124  17.981  1.00 21.20           C
ATOM   1265  OD1 ASN A 171      32.637  11.724  18.963  1.00 21.35           O
ATOM   1266  ND2 ASN A 171      33.263   9.830  17.962  1.00 19.36           N
ATOM   1267  N   LYS A 172      33.529  14.097  14.400  1.00 22.97           N
ATOM   1268  CA  LYS A 172      34.218  14.847  13.353  1.00 24.09           C
ATOM   1269  C   LYS A 172      34.167  16.342  13.656  1.00 23.61           C
ATOM   1270  O   LYS A 172      35.166  17.041  13.511  1.00 23.54           O
ATOM   1271  CB  LYS A 172      33.669  14.529  11.961  1.00 24.58           C
ATOM   1272  CG  LYS A 172      34.087  13.163  11.491  1.00 27.56           C
ATOM   1273  CD  LYS A 172      33.653  12.852  10.034  1.00 31.03           C
ATOM   1274  CE  LYS A 172      34.323  11.576   9.565  1.00 33.01           C
ATOM   1275  NZ  LYS A 172      34.357  11.406   8.070  1.00 36.89           N
ATOM   1276  N   GLN A 173      33.019  16.834  14.109  1.00 23.74           N
ATOM   1277  CA  GLN A 173      32.914  18.245  14.482  1.00 23.87           C
ATOM   1278  C   GLN A 173      33.960  18.578  15.547  1.00 23.86           C
ATOM   1279  O   GLN A 173      34.739  19.500  15.374  1.00 24.25           O
ATOM   1280  CB  GLN A 173      31.517  18.590  14.993  1.00 23.63           C
ATOM   1281  CG  GLN A 173      30.451  18.619  13.916  1.00 24.53           C
ATOM   1282  CD  GLN A 173      30.753  19.634  12.851  1.00 25.08           C
ATOM   1283  OE1 GLN A 173      31.194  20.740  13.157  1.00 26.69           O
ATOM   1284  NE2 GLN A 173      30.512  19.273  11.601  1.00 23.36           N
ATOM   1285  N   GLN A 174      33.963  17.822  16.635  1.00 23.63           N
ATOM   1286  CA  GLN A 174      34.925  17.995  17.717  1.00 23.91           C
ATOM   1287  C   GLN A 174      36.365  18.053  17.161  1.00 24.01           C
ATOM   1288  O   GLN A 174      37.133  18.962  17.480  1.00 23.39           O
ATOM   1289  CB  GLN A 174      34.783  16.840  18.717  1.00 23.67           C
ATOM   1290  CG  GLN A 174      35.688  16.913  19.934  1.00 24.07           C
ATOM   1291  CD  GLN A 174      35.595  15.668  20.799  1.00 25.12           C
ATOM   1292  OE1 GLN A 174      35.229  14.602  20.312  1.00 25.70           O
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1293 | NE2 | GLN | A | 174 | 35.901 | 15.803 | 22.084 | 1.00 | 23.63 | N |
| ATOM | 1294 | N | GLY | A | 175 | 36.706 | 17.080 | 16.334 | 1.00 | 23.75 | N |
| ATOM | 1295 | CA | GLY | A | 175 | 38.005 | 17.028 | 15.696 | 1.00 | 24.73 | C |
| ATOM | 1296 | C | GLY | A | 175 | 38.268 | 18.209 | 14.768 | 1.00 | 25.21 | C |
| ATOM | 1297 | O | GLY | A | 175 | 39.310 | 18.842 | 14.854 | 1.00 | 25.60 | O |
| ATOM | 1298 | N | LYS | A | 176 | 37.327 | 18.518 | 13.888 | 1.00 | 25.81 | N |
| ATOM | 1299 | CA | LYS | A | 176 | 37.491 | 19.634 | 12.961 | 1.00 | 26.88 | C |
| ATOM | 1300 | C | LYS | A | 176 | 37.719 | 20.997 | 13.638 | 1.00 | 26.95 | C |
| ATOM | 1301 | O | LYS | A | 176 | 38.490 | 21.803 | 13.136 | 1.00 | 26.74 | O |
| ATOM | 1302 | CB | LYS | A | 176 | 36.256 | 19.778 | 12.077 | 1.00 | 27.35 | C |
| ATOM | 1303 | CG | LYS | A | 176 | 36.093 | 18.716 | 11.009 | 1.00 | 29.87 | C |
| ATOM | 1304 | CD | LYS | A | 176 | 34.894 | 19.085 | 10.137 | 1.00 | 33.21 | C |
| ATOM | 1305 | CE | LYS | A | 176 | 33.948 | 17.932 | 9.961 | 1.00 | 35.30 | C |
| ATOM | 1306 | NZ | LYS | A | 176 | 32.558 | 18.388 | 9.643 | 1.00 | 37.22 | N |
| ATOM | 1307 | N | ARG | A | 177 | 37.031 | 21.257 | 14.749 | 1.00 | 26.93 | N |
| ATOM | 1308 | CA | ARG | A | 177 | 37.153 | 22.539 | 15.435 | 1.00 | 27.36 | C |
| ATOM | 1309 | C | ARG | A | 177 | 38.241 | 22.611 | 16.509 | 1.00 | 26.63 | C |
| ATOM | 1310 | O | ARG | A | 177 | 38.402 | 23.650 | 17.135 | 1.00 | 25.85 | O |
| ATOM | 1311 | CB | ARG | A | 177 | 35.832 | 22.902 | 16.114 | 1.00 | 27.86 | C |
| ATOM | 1312 | CG | ARG | A | 177 | 34.625 | 22.712 | 15.267 | 1.00 | 29.88 | C |
| ATOM | 1313 | CD | ARG | A | 177 | 34.653 | 23.460 | 13.973 | 1.00 | 32.39 | C |
| ATOM | 1314 | NE | ARG | A | 177 | 33.683 | 22.854 | 13.084 | 1.00 | 34.54 | N |
| ATOM | 1315 | CZ | ARG | A | 177 | 33.841 | 22.701 | 11.790 | 1.00 | 37.31 | C |
| ATOM | 1316 | NH1 | ARG | A | 177 | 34.952 | 23.110 | 11.189 | 1.00 | 38.34 | N |
| ATOM | 1317 | NH2 | ARG | A | 177 | 32.877 | 22.126 | 11.088 | 1.00 | 38.88 | N |
| ATOM | 1318 | N | GLY | A | 178 | 38.950 | 21.510 | 16.743 | 1.00 | 26.35 | N |
| ATOM | 1319 | CA | GLY | A | 178 | 39.998 | 21.470 | 17.753 | 1.00 | 25.46 | C |
| ATOM | 1320 | C | GLY | A | 178 | 39.473 | 21.514 | 19.176 | 1.00 | 25.27 | C |
| ATOM | 1321 | O | GLY | A | 178 | 40.213 | 21.818 | 20.123 | 1.00 | 25.46 | O |
| ATOM | 1322 | N | TRP | A | 179 | 38.199 | 21.202 | 19.359 | 1.00 | 24.30 | N |
| ATOM | 1323 | CA | TRP | A | 179 | 37.639 | 21.260 | 20.692 | 1.00 | 24.02 | C |
| ATOM | 1324 | C | TRP | A | 179 | 38.290 | 20.266 | 21.638 | 1.00 | 23.85 | C |
| ATOM | 1325 | O | TRP | A | 179 | 38.958 | 19.333 | 21.226 | 1.00 | 22.62 | O |
| ATOM | 1326 | CB | TRP | A | 179 | 36.136 | 21.011 | 20.674 | 1.00 | 23.73 | C |
| ATOM | 1327 | CG | TRP | A | 179 | 35.346 | 22.061 | 19.962 | 1.00 | 23.92 | C |
| ATOM | 1328 | CD1 | TRP | A | 179 | 35.787 | 23.291 | 19.531 | 1.00 | 22.69 | C |
| ATOM | 1329 | CD2 | TRP | A | 179 | 33.968 | 21.981 | 19.594 | 1.00 | 23.74 | C |
| ATOM | 1330 | NE1 | TRP | A | 179 | 34.765 | 23.968 | 18.912 | 1.00 | 24.45 | N |
| ATOM | 1331 | CE2 | TRP | A | 179 | 33.636 | 23.183 | 18.929 | 1.00 | 24.47 | C |
| ATOM | 1332 | CE3 | TRP | A | 179 | 32.984 | 21.002 | 19.730 | 1.00 | 23.10 | C |
| ATOM | 1333 | CZ2 | TRP | A | 179 | 32.379 | 23.422 | 18.414 | 1.00 | 23.69 | C |
| ATOM | 1334 | CZ3 | TRP | A | 179 | 31.733 | 21.241 | 19.211 | 1.00 | 21.89 | C |
| ATOM | 1335 | CH2 | TRP | A | 179 | 31.435 | 22.445 | 18.573 | 1.00 | 23.90 | C |
| ATOM | 1336 | N | GLY | A | 180 | 38.080 | 20.499 | 22.925 | 1.00 | 24.08 | N |
| ATOM | 1337 | CA | GLY | A | 180 | 38.488 | 19.558 | 23.941 | 1.00 | 24.08 | C |
| ATOM | 1338 | C | GLY | A | 180 | 37.437 | 18.476 | 24.103 | 1.00 | 24.64 | C |
| ATOM | 1339 | O | GLY | A | 180 | 36.618 | 18.234 | 23.202 | 1.00 | 24.66 | O |
| ATOM | 1340 | N | GLN | A | 181 | 37.437 | 17.830 | 25.261 | 1.00 | 24.77 | N |
| ATOM | 1341 | CA | GLN | A | 181 | 36.575 | 16.682 | 25.471 | 1.00 | 25.23 | C |
| ATOM | 1342 | C | GLN | A | 181 | 35.117 | 17.039 | 25.725 | 1.00 | 24.50 | C |
| ATOM | 1343 | O | GLN | A | 181 | 34.779 | 18.151 | 26.149 | 1.00 | 24.42 | O |
| ATOM | 1344 | CB | GLN | A | 181 | 37.094 | 15.847 | 26.646 | 1.00 | 25.76 | C |
| ATOM | 1345 | CG | GLN | A | 181 | 36.720 | 16.409 | 28.025 | 1.00 | 28.85 | C |
| ATOM | 1346 | CD | GLN | A | 181 | 37.046 | 15.434 | 29.156 | 1.00 | 33.38 | C |
| ATOM | 1347 | OE1 | GLN | A | 181 | 38.186 | 15.003 | 29.293 | 1.00 | 36.10 | O |
| ATOM | 1348 | NE2 | GLN | A | 181 | 36.044 | 15.085 | 29.958 | 1.00 | 36.04 | N |
| ATOM | 1349 | N | LEU | A | 182 | 34.262 | 16.078 | 25.423 | 1.00 | 23.71 | N |
| ATOM | 1350 | CA | LEU | A | 182 | 32.857 | 16.110 | 25.792 | 1.00 | 23.70 | C |
| ATOM | 1351 | C | LEU | A | 182 | 32.876 | 16.040 | 27.317 | 1.00 | 22.68 | C |
| ATOM | 1352 | O | LEU | A | 182 | 33.406 | 15.079 | 27.849 | 1.00 | 21.72 | O |
| ATOM | 1353 | CB | LEU | A | 182 | 32.179 | 14.836 | 25.273 | 1.00 | 23.82 | C |

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ATOM   1354  CG  LEU A 182      30.661  14.693  25.199  1.00 26.38           C
ATOM   1355  CD1 LEU A 182      30.243  13.231  25.368  1.00 26.04           C
ATOM   1356  CD2 LEU A 182      29.977  15.501  26.192  1.00 29.73           C
ATOM   1357  N   THR A 183      32.323  17.031  28.021  1.00 21.93           N
ATOM   1358  CA  THR A 183      32.300  16.971  29.484  1.00 21.44           C
ATOM   1359  C   THR A 183      31.004  16.388  29.984  1.00 21.27           C
ATOM   1360  O   THR A 183      30.972  15.766  31.032  1.00 21.29           O
ATOM   1361  CB  THR A 183      32.490  18.362  30.150  1.00 21.73           C
ATOM   1362  OG1 THR A 183      31.463  19.257  29.715  1.00 20.35           O
ATOM   1363  CG2 THR A 183      33.796  19.015  29.725  1.00 20.91           C
ATOM   1364  N   SER A 184      29.918  16.590  29.251  1.00 21.42           N
ATOM   1365  CA  SER A 184      28.649  16.053  29.689  1.00 21.45           C
ATOM   1366  C   SER A 184      27.537  16.272  28.714  1.00 21.46           C
ATOM   1367  O   SER A 184      27.672  17.031  27.753  1.00 21.17           O
ATOM   1368  CB  SER A 184      28.243  16.687  31.006  1.00 21.74           C
ATOM   1369  OG  SER A 184      27.919  18.049  30.845  1.00 23.24           O
ATOM   1370  N   ASN A 185      26.445  15.575  28.982  1.00 21.21           N
ATOM   1371  CA  ASN A 185      25.216  15.712  28.245  1.00 22.29           C
ATOM   1372  C   ASN A 185      24.154  16.005  29.273  1.00 22.08           C
ATOM   1373  O   ASN A 185      23.886  15.184  30.135  1.00 22.25           O
ATOM   1374  CB  ASN A 185      24.856  14.416  27.497  1.00 22.67           C
ATOM   1375  CG  ASN A 185      25.885  14.037  26.454  1.00 23.57           C
ATOM   1376  OD1 ASN A 185      26.646  13.097  26.655  1.00 27.51           O
ATOM   1377  ND2 ASN A 185      25.905  14.754  25.329  1.00 24.27           N
ATOM   1378  N   LEU A 186      23.574  17.189  29.202  1.00 22.01           N
ATOM   1379  CA  LEU A 186      22.529  17.563  30.135  1.00 22.03           C
ATOM   1380  C   LEU A 186      21.170  17.219  29.558  1.00 22.00           C
ATOM   1381  O   LEU A 186      20.844  17.592  28.435  1.00 22.34           O
ATOM   1382  CB  LEU A 186      22.578  19.065  30.423  1.00 21.68           C
ATOM   1383  CG  LEU A 186      21.707  19.538  31.588  1.00 22.25           C
ATOM   1384  CD1 LEU A 186      22.252  18.985  32.891  1.00 22.43           C
ATOM   1385  CD2 LEU A 186      21.643  21.098  31.648  1.00 23.35           C
ATOM   1386  N   LEU A 187      20.377  16.518  30.344  1.00 22.19           N
ATOM   1387  CA  LEU A 187      19.009  16.198  29.979  1.00 21.95           C
ATOM   1388  C   LEU A 187      18.149  17.286  30.603  1.00 21.91           C
ATOM   1389  O   LEU A 187      18.232  17.521  31.823  1.00 21.61           O
ATOM   1390  CB  LEU A 187      18.616  14.830  30.527  1.00 21.55           C
ATOM   1391  CG  LEU A 187      17.129  14.488  30.477  1.00 22.78           C
ATOM   1392  CD1 LEU A 187      16.616  14.429  29.054  1.00 23.66           C
ATOM   1393  CD2 LEU A 187      16.866  13.143  31.174  1.00 22.84           C
ATOM   1394  N   LEU A 188      17.348  17.956  29.770  1.00 21.56           N
ATOM   1395  CA  LEU A 188      16.461  19.000  30.227  1.00 22.26           C
ATOM   1396  C   LEU A 188      14.993  18.662  29.920  1.00 22.55           C
ATOM   1397  O   LEU A 188      14.588  18.517  28.760  1.00 23.16           O
ATOM   1398  CB  LEU A 188      16.827  20.327  29.562  1.00 22.84           C
ATOM   1399  CG  LEU A 188      18.244  20.840  29.821  1.00 22.60           C
ATOM   1400  CD1 LEU A 188      18.967  21.111  28.523  1.00 23.92           C
ATOM   1401  CD2 LEU A 188      18.177  22.088  30.655  1.00 24.56           C
ATOM   1402  N   ILE A 189      14.181  18.577  30.958  1.00 22.15           N
ATOM   1403  CA  ILE A 189      12.769  18.315  30.756  1.00 22.34           C
ATOM   1404  C   ILE A 189      11.996  19.395  31.460  1.00 22.37           C
ATOM   1405  O   ILE A 189      12.072  19.528  32.692  1.00 22.77           O
ATOM   1406  CB  ILE A 189      12.377  16.953  31.281  1.00 21.60           C
ATOM   1407  CG1 ILE A 189      13.254  15.888  30.638  1.00 21.85           C
ATOM   1408  CG2 ILE A 189      10.928  16.708  30.958  1.00 22.51           C
ATOM   1409  CD1 ILE A 189      12.918  14.425  31.075  1.00 23.06           C
ATOM   1410  N   GLY A 190      11.276  20.186  30.673  1.00 22.37           N
ATOM   1411  CA  GLY A 190      10.587  21.336  31.206  1.00 22.29           C
ATOM   1412  C   GLY A 190       9.124  21.342  30.902  1.00 22.48           C
ATOM   1413  O   GLY A 190       8.652  20.633  30.007  1.00 22.39           O
ATOM   1414  N   MET A 191       8.402  22.134  31.687  1.00 22.74           N
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1415 | CA | MET | A | 191 | 6.991 | 22.339 | 31.467 | 1.00 | 23.16 | C |
| ATOM | 1416 | C | MET | A | 191 | 6.838 | 23.482 | 30.478 | 1.00 | 22.94 | C |
| ATOM | 1417 | O | MET | A | 191 | 7.738 | 24.329 | 30.338 | 1.00 | 23.03 | O |
| ATOM | 1418 | CB | MET | A | 191 | 6.283 | 22.673 | 32.784 | 1.00 | 23.69 | C |
| ATOM | 1419 | CG | MET | A | 191 | 6.224 | 21.513 | 33.741 | 1.00 | 25.02 | C |
| ATOM | 1420 | SD | MET | A | 191 | 5.664 | 21.927 | 35.415 | 1.00 | 28.11 | S |
| ATOM | 1421 | CE | MET | A | 191 | 4.016 | 22.460 | 35.097 | 1.00 | 28.35 | C |
| ATOM | 1422 | N | GLU | A | 192 | 5.712 | 23.492 | 29.773 | 1.00 | 22.60 | N |
| ATOM | 1423 | CA | GLU | A | 192 | 5.410 | 24.544 | 28.810 | 1.00 | 22.83 | C |
| ATOM | 1424 | C | GLU | A | 192 | 5.495 | 25.895 | 29.490 | 1.00 | 22.51 | C |
| ATOM | 1425 | O | GLU | A | 192 | 5.062 | 26.046 | 30.614 | 1.00 | 22.41 | O |
| ATOM | 1426 | CB | GLU | A | 192 | 4.005 | 24.342 | 28.249 | 1.00 | 22.86 | C |
| ATOM | 1427 | CG | GLU | A | 192 | 2.925 | 24.367 | 29.315 | 1.00 | 24.36 | C |
| ATOM | 1428 | CD | GLU | A | 192 | 1.572 | 23.891 | 28.814 | 1.00 | 25.71 | C |
| ATOM | 1429 | OE1 | GLU | A | 192 | 1.503 | 23.294 | 27.718 | 1.00 | 25.51 | O |
| ATOM | 1430 | OE2 | GLU | A | 192 | 0.582 | 24.128 | 29.525 | 1.00 | 26.30 | O |
| ATOM | 1431 | N | GLY | A | 193 | 6.069 | 26.888 | 28.828 | 1.00 | 22.95 | N |
| ATOM | 1432 | CA | GLY | A | 193 | 6.185 | 28.199 | 29.444 | 1.00 | 22.50 | C |
| ATOM | 1433 | C | GLY | A | 193 | 7.465 | 28.414 | 30.254 | 1.00 | 22.36 | C |
| ATOM | 1434 | O | GLY | A | 193 | 7.756 | 29.544 | 30.602 | 1.00 | 23.08 | O |
| ATOM | 1435 | N | ASN | A | 194 | 8.219 | 27.361 | 30.566 | 1.00 | 21.60 | N |
| ATOM | 1436 | CA | ASN | A | 194 | 9.456 | 27.506 | 31.341 | 1.00 | 21.44 | C |
| ATOM | 1437 | C | ASN | A | 194 | 10.489 | 28.320 | 30.581 | 1.00 | 21.19 | C |
| ATOM | 1438 | O | ASN | A | 194 | 10.635 | 28.134 | 29.372 | 1.00 | 22.08 | O |
| ATOM | 1439 | CB | ASN | A | 194 | 10.099 | 26.147 | 31.629 | 1.00 | 21.05 | C |
| ATOM | 1440 | CG | ASN | A | 194 | 9.494 | 25.435 | 32.801 | 1.00 | 20.86 | C |
| ATOM | 1441 | OD1 | ASN | A | 194 | 8.509 | 25.883 | 33.385 | 1.00 | 22.48 | O |
| ATOM | 1442 | ND2 | ASN | A | 194 | 10.092 | 24.312 | 33.167 | 1.00 | 17.74 | N |
| ATOM | 1443 | N | VAL | A | 195 | 11.213 | 29.183 | 31.290 | 1.00 | 20.69 | N |
| ATOM | 1444 | CA | VAL | A | 195 | 12.268 | 29.993 | 30.701 | 1.00 | 20.84 | C |
| ATOM | 1445 | C | VAL | A | 195 | 13.572 | 29.854 | 31.450 | 1.00 | 20.06 | C |
| ATOM | 1446 | O | VAL | A | 195 | 13.601 | 29.874 | 32.681 | 1.00 | 20.75 | O |
| ATOM | 1447 | CB | VAL | A | 195 | 11.903 | 31.502 | 30.686 | 1.00 | 21.41 | C |
| ATOM | 1448 | CG1 | VAL | A | 195 | 13.081 | 32.357 | 30.219 | 1.00 | 22.24 | C |
| ATOM | 1449 | CG2 | VAL | A | 195 | 10.666 | 31.767 | 29.843 | 1.00 | 22.30 | C |
| ATOM | 1450 | N | THR | A | 196 | 14.651 | 29.673 | 30.702 | 1.00 | 19.51 | N |
| ATOM | 1451 | CA | THR | A | 196 | 15.993 | 29.737 | 31.257 | 1.00 | 19.52 | C |
| ATOM | 1452 | C | THR | A | 196 | 16.487 | 31.117 | 30.820 | 1.00 | 19.98 | C |
| ATOM | 1453 | O | THR | A | 196 | 16.653 | 31.352 | 29.620 | 1.00 | 19.56 | O |
| ATOM | 1454 | CB | THR | A | 196 | 16.896 | 28.677 | 30.675 | 1.00 | 19.26 | C |
| ATOM | 1455 | OG1 | THR | A | 196 | 16.526 | 27.366 | 31.162 | 1.00 | 21.13 | O |
| ATOM | 1456 | CG2 | THR | A | 196 | 18.309 | 28.886 | 31.185 | 1.00 | 19.85 | C |
| ATOM | 1457 | N | PRO | A | 197 | 16.627 | 32.043 | 31.767 | 1.00 | 20.27 | N |
| ATOM | 1458 | CA | PRO | A | 197 | 17.046 | 33.412 | 31.463 | 1.00 | 20.52 | C |
| ATOM | 1459 | C | PRO | A | 197 | 18.431 | 33.497 | 30.836 | 1.00 | 20.89 | C |
| ATOM | 1460 | O | PRO | A | 197 | 19.277 | 32.609 | 31.025 | 1.00 | 20.66 | O |
| ATOM | 1461 | CB | PRO | A | 197 | 17.018 | 34.099 | 32.825 | 1.00 | 21.22 | C |
| ATOM | 1462 | CG | PRO | A | 197 | 16.144 | 33.263 | 33.657 | 1.00 | 21.01 | C |
| ATOM | 1463 | CD | PRO | A | 197 | 16.309 | 31.872 | 33.189 | 1.00 | 20.28 | C |
| ATOM | 1464 | N | ALA | A | 198 | 18.633 | 34.577 | 30.089 | 1.00 | 20.28 | N |
| ATOM | 1465 | CA | ALA | A | 198 | 19.841 | 34.817 | 29.341 | 1.00 | 20.22 | C |
| ATOM | 1466 | C | ALA | A | 198 | 21.130 | 34.634 | 30.146 | 1.00 | 20.58 | C |
| ATOM | 1467 | O | ALA | A | 198 | 21.284 | 35.186 | 31.235 | 1.00 | 19.91 | O |
| ATOM | 1468 | CB | ALA | A | 198 | 19.791 | 36.222 | 28.759 | 1.00 | 20.52 | C |
| ATOM | 1469 | N | HIS | A | 199 | 22.062 | 33.891 | 29.563 | 1.00 | 20.87 | N |
| ATOM | 1470 | CA | HIS | A | 199 | 23.371 | 33.646 | 30.158 | 1.00 | 21.41 | C |
| ATOM | 1471 | C | HIS | A | 199 | 24.281 | 33.168 | 29.063 | 1.00 | 21.82 | C |
| ATOM | 1472 | O | HIS | A | 199 | 23.826 | 32.892 | 27.943 | 1.00 | 21.80 | O |
| ATOM | 1473 | CB | HIS | A | 199 | 23.305 | 32.534 | 31.198 | 1.00 | 21.44 | C |
| ATOM | 1474 | CG | HIS | A | 199 | 22.915 | 31.220 | 30.617 | 1.00 | 22.21 | C |
| ATOM | 1475 | ND1 | HIS | A | 199 | 21.619 | 30.940 | 30.253 | 1.00 | 21.93 | N |

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ATOM   1476  CD2 HIS A 199      23.644  30.120  30.296  1.00 22.04           C
ATOM   1477  CE1 HIS A 199      21.561  29.721  29.749  1.00 23.76           C
ATOM   1478  NE2 HIS A 199      22.777  29.214  29.737  1.00 22.57           N
ATOM   1479  N   TYR A 200      25.568  33.060  29.384  1.00 22.40           N
ATOM   1480  CA  TYR A 200      26.536  32.456  28.469  1.00 22.34           C
ATOM   1481  C   TYR A 200      27.225  31.316  29.197  1.00 22.03           C
ATOM   1482  O   TYR A 200      27.328  31.330  30.425  1.00 21.90           O
ATOM   1483  CB  TYR A 200      27.544  33.458  27.924  1.00 22.22           C
ATOM   1484  CG  TYR A 200      28.517  34.051  28.924  1.00 22.16           C
ATOM   1485  CD1 TYR A 200      29.746  33.454  29.171  1.00 21.36           C
ATOM   1486  CD2 TYR A 200      28.236  35.246  29.565  1.00 22.58           C
ATOM   1487  CE1 TYR A 200      30.638  33.997  30.052  1.00 21.48           C
ATOM   1488  CE2 TYR A 200      29.128  35.806  30.462  1.00 21.46           C
ATOM   1489  CZ  TYR A 200      30.334  35.189  30.695  1.00 22.03           C
ATOM   1490  OH  TYR A 200      31.230  35.733  31.593  1.00 20.69           O
ATOM   1491  N   ASP A 201      27.681  30.310  28.444  1.00 22.42           N
ATOM   1492  CA  ASP A 201      28.381  29.152  29.048  1.00 22.10           C
ATOM   1493  C   ASP A 201      29.801  29.142  28.531  1.00 21.96           C
ATOM   1494  O   ASP A 201      30.018  29.601  27.433  1.00 22.26           O
ATOM   1495  CB  ASP A 201      27.722  27.840  28.661  1.00 21.97           C
ATOM   1496  CG  ASP A 201      26.311  27.714  29.181  1.00 21.99           C
ATOM   1497  OD1 ASP A 201      26.126  27.649  30.421  1.00 22.61           O
ATOM   1498  OD2 ASP A 201      25.330  27.624  28.412  1.00 19.35           O
ATOM   1499  N   GLU A 202      30.769  28.620  29.283  1.00 21.66           N
ATOM   1500  CA  GLU A 202      32.146  28.612  28.773  1.00 23.16           C
ATOM   1501  C   GLU A 202      32.515  27.334  28.035  1.00 23.38           C
ATOM   1502  O   GLU A 202      33.684  26.951  28.049  1.00 25.48           O
ATOM   1503  CB  GLU A 202      33.178  28.774  29.897  1.00 23.46           C
ATOM   1504  CG  GLU A 202      33.110  30.064  30.681  1.00 26.52           C
ATOM   1505  CD  GLU A 202      34.233  30.132  31.704  1.00 28.11           C
ATOM   1506  OE1 GLU A 202      34.207  29.387  32.698  1.00 29.06           O
ATOM   1507  OE2 GLU A 202      35.148  30.920  31.490  1.00 31.04           O
ATOM   1508  N   GLN A 203      31.538  26.632  27.476  1.00 22.70           N
ATOM   1509  CA  GLN A 203      31.808  25.451  26.685  1.00 22.01           C
ATOM   1510  C   GLN A 203      31.049  25.576  25.373  1.00 21.93           C
ATOM   1511  O   GLN A 203      30.113  26.378  25.253  1.00 22.49           O
ATOM   1512  CB  GLN A 203      31.409  24.169  27.427  1.00 22.02           C
ATOM   1513  CG  GLN A 203      32.287  23.822  28.657  1.00 22.33           C
ATOM   1514  CD  GLN A 203      32.103  22.379  29.165  1.00 23.14           C
ATOM   1515  OE1 GLN A 203      31.948  21.448  28.370  1.00 21.46           O
ATOM   1516  NE2 GLN A 203      32.138  22.203  30.489  1.00 21.21           N
ATOM   1517  N   GLN A 204      31.486  24.807  24.380  1.00 21.81           N
ATOM   1518  CA  GLN A 204      30.806  24.720  23.092  1.00 21.45           C
ATOM   1519  C   GLN A 204      29.610  23.799  23.295  1.00 21.12           C
ATOM   1520  O   GLN A 204      29.673  22.862  24.088  1.00 20.29           O
ATOM   1521  CB  GLN A 204      31.740  24.140  22.040  1.00 21.75           C
ATOM   1522  CG  GLN A 204      33.033  24.928  21.852  1.00 21.56           C
ATOM   1523  CD  GLN A 204      32.856  26.198  21.000  1.00 21.57           C
ATOM   1524  OE1 GLN A 204      31.741  26.609  20.692  1.00 20.30           O
ATOM   1525  NE2 GLN A 204      33.966  26.776  20.594  1.00 18.60           N
ATOM   1526  N   ASN A 205      28.522  24.060  22.580  1.00 21.25           N
ATOM   1527  CA  ASN A 205      27.291  23.316  22.795  1.00 21.04           C
ATOM   1528  C   ASN A 205      26.529  22.977  21.526  1.00 21.25           C
ATOM   1529  O   ASN A 205      26.160  23.880  20.747  1.00 20.22           O
ATOM   1530  CB  ASN A 205      26.387  24.194  23.654  1.00 21.95           C
ATOM   1531  CG  ASN A 205      25.116  23.507  24.098  1.00 21.98           C
ATOM   1532  OD1 ASN A 205      24.759  22.418  23.643  1.00 21.21           O
ATOM   1533  ND2 ASN A 205      24.400  24.178  24.979  1.00 17.72           N
ATOM   1534  N   PHE A 206      26.314  21.677  21.319  1.00 19.90           N
ATOM   1535  CA  PHE A 206      25.339  21.230  20.354  1.00 19.77           C
ATOM   1536  C   PHE A 206      24.085  20.869  21.150  1.00 19.25           C
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ATOM   1537  O   PHE A 206      24.094  19.939  21.959  1.00 19.15           O
ATOM   1538  CB  PHE A 206      25.849  20.049  19.545  1.00 20.09           C
ATOM   1539  CG  PHE A 206      26.786  20.442  18.454  1.00 19.77           C
ATOM   1540  CD1 PHE A 206      26.371  21.294  17.453  1.00 22.21           C
ATOM   1541  CD2 PHE A 206      28.079  19.973  18.435  1.00 20.21           C
ATOM   1542  CE1 PHE A 206      27.213  21.643  16.434  1.00 22.06           C
ATOM   1543  CE2 PHE A 206      28.941  20.336  17.418  1.00 20.66           C
ATOM   1544  CZ  PHE A 206      28.504  21.190  16.427  1.00 22.18           C
ATOM   1545  N   PHE A 207      23.009  21.596  20.869  1.00 18.42           N
ATOM   1546  CA  PHE A 207      21.760  21.590  21.620  1.00 18.78           C
ATOM   1547  C   PHE A 207      20.732  20.841  20.804  1.00 19.36           C
ATOM   1548  O   PHE A 207      20.241  21.359  19.818  1.00 19.26           O
ATOM   1549  CB  PHE A 207      21.366  23.063  21.836  1.00 18.70           C
ATOM   1550  CG  PHE A 207      20.120  23.301  22.635  1.00 17.94           C
ATOM   1551  CD1 PHE A 207      18.899  23.404  22.007  1.00 17.78           C
ATOM   1552  CD2 PHE A 207      20.188  23.548  23.989  1.00 18.50           C
ATOM   1553  CE1 PHE A 207      17.772  23.684  22.713  1.00 19.52           C
ATOM   1554  CE2 PHE A 207      19.052  23.823  24.705  1.00 20.66           C
ATOM   1555  CZ  PHE A 207      17.836  23.909  24.053  1.00 19.44           C
ATOM   1556  N   ALA A 208      20.435  19.618  21.234  1.00 19.90           N
ATOM   1557  CA  ALA A 208      19.628  18.670  20.469  1.00 20.17           C
ATOM   1558  C   ALA A 208      18.210  18.541  20.991  1.00 20.52           C
ATOM   1559  O   ALA A 208      17.971  17.946  22.047  1.00 20.61           O
ATOM   1560  CB  ALA A 208      20.294  17.308  20.494  1.00 19.33           C
ATOM   1561  N   GLN A 209      17.270  19.076  20.219  1.00 20.94           N
ATOM   1562  CA  GLN A 209      15.880  19.062  20.627  1.00 20.82           C
ATOM   1563  C   GLN A 209      15.227  17.712  20.323  1.00 20.75           C
ATOM   1564  O   GLN A 209      15.401  17.129  19.224  1.00 19.59           O
ATOM   1565  CB  GLN A 209      15.141  20.216  19.961  1.00 20.91           C
ATOM   1566  CG  GLN A 209      13.735  20.431  20.463  1.00 20.52           C
ATOM   1567  CD  GLN A 209      13.673  20.840  21.928  1.00 20.69           C
ATOM   1568  OE1 GLN A 209      14.702  21.155  22.562  1.00 19.72           O
ATOM   1569  NE2 GLN A 209      12.460  20.852  22.473  1.00 19.21           N
ATOM   1570  N   ILE A 210      14.442  17.248  21.296  1.00 20.72           N
ATOM   1571  CA  ILE A 210      13.853  15.922  21.252  1.00 21.43           C
ATOM   1572  C   ILE A 210      12.334  15.911  21.292  1.00 21.72           C
ATOM   1573  O   ILE A 210      11.728  15.195  20.534  1.00 22.12           O
ATOM   1574  CB  ILE A 210      14.396  15.095  22.424  1.00 21.84           C
ATOM   1575  CG1 ILE A 210      15.859  14.733  22.156  1.00 22.48           C
ATOM   1576  CG2 ILE A 210      13.581  13.832  22.622  1.00 21.83           C
ATOM   1577  CD1 ILE A 210      16.631  14.354  23.382  1.00 24.34           C
ATOM   1578  N   LYS A 211      11.728  16.677  22.188  1.00 22.08           N
ATOM   1579  CA  LYS A 211      10.279  16.715  22.319  1.00 21.72           C
ATOM   1580  C   LYS A 211       9.858  18.130  22.564  1.00 21.67           C
ATOM   1581  O   LYS A 211      10.468  18.841  23.372  1.00 20.87           O
ATOM   1582  CB  LYS A 211       9.797  15.856  23.487  1.00 22.44           C
ATOM   1583  CG  LYS A 211       8.267  15.562  23.479  1.00 23.29           C
ATOM   1584  CD  LYS A 211       7.791  15.022  24.824  1.00 25.02           C
ATOM   1585  CE  LYS A 211       6.494  14.215  24.757  1.00 26.00           C
ATOM   1586  NZ  LYS A 211       5.561  14.522  23.634  1.00 26.43           N
ATOM   1587  N   GLY A 212       8.798  18.541  21.875  1.00 21.35           N
ATOM   1588  CA  GLY A 212       8.306  19.891  21.994  1.00 21.71           C
ATOM   1589  C   GLY A 212       9.195  20.906  21.297  1.00 21.63           C
ATOM   1590  O   GLY A 212      10.150  20.572  20.591  1.00 21.32           O
ATOM   1591  N   TYR A 213       8.871  22.166  21.522  1.00 22.35           N
ATOM   1592  CA  TYR A 213       9.533  23.279  20.862  1.00 22.42           C
ATOM   1593  C   TYR A 213      10.028  24.293  21.868  1.00 22.33           C
ATOM   1594  O   TYR A 213       9.340  24.589  22.853  1.00 21.55           O
ATOM   1595  CB  TYR A 213       8.556  23.951  19.916  1.00 23.46           C
ATOM   1596  CG  TYR A 213       8.114  23.034  18.815  1.00 24.81           C
ATOM   1597  CD1 TYR A 213       7.100  22.112  19.020  1.00 28.16           C
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ATOM   1598  CD2 TYR A 213       8.751  23.051  17.589  1.00 26.74           C
ATOM   1599  CE1 TYR A 213       6.716  21.237  18.011  1.00 28.91           C
ATOM   1600  CE2 TYR A 213       8.378  22.193  16.585  1.00 28.63           C
ATOM   1601  CZ  TYR A 213       7.366  21.295  16.795  1.00 29.44           C
ATOM   1602  OH  TYR A 213       7.013  20.456  15.756  1.00 33.67           O
ATOM   1603  N   LYS A 214      11.239  24.788  21.609  1.00 21.60           N
ATOM   1604  CA  LYS A 214      11.875  25.793  22.414  1.00 21.89           C
ATOM   1605  C   LYS A 214      12.312  26.947  21.528  1.00 21.62           C
ATOM   1606  O   LYS A 214      12.878  26.747  20.442  1.00 22.07           O
ATOM   1607  CB  LYS A 214      13.103  25.239  23.140  1.00 22.10           C
ATOM   1608  CG  LYS A 214      12.796  24.385  24.338  1.00 22.63           C
ATOM   1609  CD  LYS A 214      14.103  23.893  24.964  1.00 24.24           C
ATOM   1610  CE  LYS A 214      13.923  23.478  26.402  1.00 23.54           C
ATOM   1611  NZ  LYS A 214      15.169  22.872  26.951  1.00 22.10           N
ATOM   1612  N   ARG A 215      12.007  28.156  21.974  1.00 20.97           N
ATOM   1613  CA  ARG A 215      12.447  29.347  21.277  1.00 20.73           C
ATOM   1614  C   ARG A 215      13.778  29.724  21.900  1.00 20.03           C
ATOM   1615  O   ARG A 215      13.885  29.828  23.113  1.00 19.70           O
ATOM   1616  CB  ARG A 215      11.461  30.470  21.493  1.00 21.30           C
ATOM   1617  CG  ARG A 215      11.754  31.760  20.726  1.00 22.21           C
ATOM   1618  CD  ARG A 215      11.177  32.925  21.473  1.00 24.71           C
ATOM   1619  NE  ARG A 215      11.122  34.156  20.715  1.00 25.47           N
ATOM   1620  CZ  ARG A 215      10.479  35.235  21.130  1.00 26.28           C
ATOM   1621  NH1 ARG A 215       9.844  35.245  22.299  1.00 26.07           N
ATOM   1622  NH2 ARG A 215      10.483  36.314  20.384  1.00 28.83           N
ATOM   1623  N   CYS A 216      14.794  29.877  21.074  1.00 19.45           N
ATOM   1624  CA  CYS A 216      16.116  30.219  21.554  1.00 19.58           C
ATOM   1625  C   CYS A 216      16.503  31.587  20.993  1.00 19.92           C
ATOM   1626  O   CYS A 216      16.503  31.774  19.789  1.00 20.16           O
ATOM   1627  CB  CYS A 216      17.110  29.186  21.073  1.00 20.01           C
ATOM   1628  SG  CYS A 216      16.693  27.450  21.462  1.00 21.39           S
ATOM   1629  N   ILE A 217      16.812  32.530  21.878  1.00 19.28           N
ATOM   1630  CA  ILE A 217      17.286  33.845  21.504  1.00 19.58           C
ATOM   1631  C   ILE A 217      18.742  33.961  21.937  1.00 19.21           C
ATOM   1632  O   ILE A 217      19.055  33.849  23.126  1.00 19.05           O
ATOM   1633  CB  ILE A 217      16.424  34.943  22.168  1.00 19.88           C
ATOM   1634  CG1 ILE A 217      14.926  34.687  21.878  1.00 20.56           C
ATOM   1635  CG2 ILE A 217      16.803  36.312  21.627  1.00 20.25           C
ATOM   1636  CD1 ILE A 217      13.984  35.692  22.488  1.00 20.99           C
ATOM   1637  N   LEU A 218      19.620  34.176  20.965  1.00 19.01           N
ATOM   1638  CA  LEU A 218      21.048  34.271  21.222  1.00 19.61           C
ATOM   1639  C   LEU A 218      21.568  35.682  20.970  1.00 20.43           C
ATOM   1640  O   LEU A 218      21.018  36.414  20.136  1.00 19.76           O
ATOM   1641  CB  LEU A 218      21.816  33.329  20.308  1.00 19.66           C
ATOM   1642  CG  LEU A 218      21.906  31.881  20.778  1.00 19.74           C
ATOM   1643  CD1 LEU A 218      20.549  31.237  20.905  1.00 20.56           C
ATOM   1644  CD2 LEU A 218      22.733  31.099  19.798  1.00 21.32           C
ATOM   1645  N   PHE A 219      22.626  36.046  21.700  1.00 20.11           N
ATOM   1646  CA  PHE A 219      23.282  37.324  21.524  1.00 20.96           C
ATOM   1647  C   PHE A 219      24.805  37.078  21.453  1.00 21.19           C
ATOM   1648  O   PHE A 219      25.351  36.313  22.257  1.00 21.20           O
ATOM   1649  CB  PHE A 219      22.942  38.304  22.678  1.00 20.97           C
ATOM   1650  CG  PHE A 219      21.463  38.456  22.954  1.00 20.44           C
ATOM   1651  CD1 PHE A 219      20.821  37.637  23.846  1.00 21.46           C
ATOM   1652  CD2 PHE A 219      20.724  39.447  22.334  1.00 22.49           C
ATOM   1653  CE1 PHE A 219      19.472  37.790  24.108  1.00 22.33           C
ATOM   1654  CE2 PHE A 219      19.387  39.605  22.605  1.00 21.32           C
ATOM   1655  CZ  PHE A 219      18.760  38.773  23.480  1.00 21.50           C
ATOM   1656  N   PRO A 220      25.485  37.705  20.498  1.00 21.20           N
ATOM   1657  CA  PRO A 220      26.936  37.541  20.368  1.00 21.72           C
ATOM   1658  C   PRO A 220      27.683  38.108  21.569  1.00 21.31           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1659 | O | PRO | A | 220 | 27.165 | 38.972 | 22.280 | 1.00 | 20.90 | O |
| ATOM | 1660 | CB | PRO | A | 220 | 27.302 | 38.341 | 19.120 | 1.00 | 21.41 | C |
| ATOM | 1661 | CG | PRO | A | 220 | 26.020 | 38.781 | 18.510 | 1.00 | 23.12 | C |
| ATOM | 1662 | CD | PRO | A | 220 | 24.938 | 38.637 | 19.508 | 1.00 | 22.22 | C |
| ATOM | 1663 | N | PRO | A | 221 | 28.884 | 37.594 | 21.806 | 1.00 | 21.46 | N |
| ATOM | 1664 | CA | PRO | A | 221 | 29.721 | 38.053 | 22.918 | 1.00 | 21.33 | C |
| ATOM | 1665 | C | PRO | A | 221 | 29.961 | 39.556 | 22.940 | 1.00 | 21.04 | C |
| ATOM | 1666 | O | PRO | A | 221 | 30.220 | 40.096 | 24.009 | 1.00 | 20.68 | O |
| ATOM | 1667 | CB | PRO | A | 221 | 31.032 | 37.325 | 22.681 | 1.00 | 21.42 | C |
| ATOM | 1668 | CG | PRO | A | 221 | 30.656 | 36.134 | 21.939 | 1.00 | 22.42 | C |
| ATOM | 1669 | CD | PRO | A | 221 | 29.522 | 36.510 | 21.041 | 1.00 | 21.53 | C |
| ATOM | 1670 | N | ASP | A | 222 | 29.877 | 40.225 | 21.792 | 1.00 | 21.47 | N |
| ATOM | 1671 | CA | ASP | A | 222 | 30.128 | 41.669 | 21.749 | 1.00 | 21.80 | C |
| ATOM | 1672 | C | ASP | A | 222 | 28.946 | 42.464 | 22.271 | 1.00 | 21.74 | C |
| ATOM | 1673 | O | ASP | A | 222 | 28.970 | 43.685 | 22.261 | 1.00 | 22.16 | O |
| ATOM | 1674 | CB | ASP | A | 222 | 30.568 | 42.148 | 20.355 | 1.00 | 21.85 | C |
| ATOM | 1675 | CG | ASP | A | 222 | 29.433 | 42.151 | 19.325 | 1.00 | 24.83 | C |
| ATOM | 1676 | OD1 | ASP | A | 222 | 28.311 | 41.668 | 19.585 | 1.00 | 25.32 | O |
| ATOM | 1677 | OD2 | ASP | A | 222 | 29.595 | 42.607 | 18.186 | 1.00 | 29.30 | O |
| ATOM | 1678 | N | GLN | A | 223 | 27.916 | 41.775 | 22.748 | 1.00 | 21.94 | N |
| ATOM | 1679 | CA | GLN | A | 223 | 26.794 | 42.453 | 23.388 | 1.00 | 22.17 | C |
| ATOM | 1680 | C | GLN | A | 223 | 26.897 | 42.388 | 24.928 | 1.00 | 21.93 | C |
| ATOM | 1681 | O | GLN | A | 223 | 25.926 | 42.681 | 25.660 | 1.00 | 21.70 | O |
| ATOM | 1682 | CB | GLN | A | 223 | 25.456 | 41.911 | 22.832 | 1.00 | 22.84 | C |
| ATOM | 1683 | CG | GLN | A | 223 | 25.149 | 42.508 | 21.412 | 1.00 | 25.34 | C |
| ATOM | 1684 | CD | GLN | A | 223 | 23.728 | 42.283 | 20.965 | 1.00 | 27.81 | C |
| ATOM | 1685 | OE1 | GLN | A | 223 | 22.801 | 42.473 | 21.750 | 1.00 | 30.00 | O |
| ATOM | 1686 | NE2 | GLN | A | 223 | 23.543 | 41.850 | 19.709 | 1.00 | 29.69 | N |
| ATOM | 1687 | N | PHE | A | 224 | 28.079 | 42.027 | 25.417 | 1.00 | 21.04 | N |
| ATOM | 1688 | CA | PHE | A | 224 | 28.363 | 42.035 | 26.860 | 1.00 | 21.41 | C |
| ATOM | 1689 | C | PHE | A | 224 | 27.886 | 43.350 | 27.527 | 1.00 | 21.57 | C |
| ATOM | 1690 | O | PHE | A | 224 | 27.240 | 43.315 | 28.561 | 1.00 | 21.34 | O |
| ATOM | 1691 | CB | PHE | A | 224 | 29.883 | 41.874 | 27.076 | 1.00 | 20.95 | C |
| ATOM | 1692 | CG | PHE | A | 224 | 30.304 | 41.773 | 28.529 | 1.00 | 21.82 | C |
| ATOM | 1693 | CD1 | PHE | A | 224 | 30.452 | 42.912 | 29.319 | 1.00 | 19.33 | C |
| ATOM | 1694 | CD2 | PHE | A | 224 | 30.595 | 40.552 | 29.089 | 1.00 | 20.01 | C |
| ATOM | 1695 | CE1 | PHE | A | 224 | 30.870 | 42.807 | 30.630 | 1.00 | 20.89 | C |
| ATOM | 1696 | CE2 | PHE | A | 224 | 31.025 | 40.449 | 30.397 | 1.00 | 20.59 | C |
| ATOM | 1697 | CZ | PHE | A | 224 | 31.151 | 41.579 | 31.171 | 1.00 | 20.99 | C |
| ATOM | 1698 | N | GLU | A | 225 | 28.195 | 44.495 | 26.916 | 1.00 | 22.10 | N |
| ATOM | 1699 | CA | GLU | A | 225 | 27.823 | 45.800 | 27.466 | 1.00 | 23.01 | C |
| ATOM | 1700 | C | GLU | A | 225 | 26.337 | 46.042 | 27.574 | 1.00 | 22.26 | C |
| ATOM | 1701 | O | GLU | A | 225 | 25.928 | 46.946 | 28.311 | 1.00 | 21.91 | O |
| ATOM | 1702 | CB | GLU | A | 225 | 28.401 | 46.935 | 26.624 | 1.00 | 24.27 | C |
| ATOM | 1703 | CG | GLU | A | 225 | 29.886 | 47.133 | 26.857 | 1.00 | 29.26 | C |
| ATOM | 1704 | CD | GLU | A | 225 | 30.312 | 48.579 | 27.062 | 1.00 | 35.91 | C |
| ATOM | 1705 | OE1 | GLU | A | 225 | 29.745 | 49.317 | 27.942 | 1.00 | 39.92 | O |
| ATOM | 1706 | OE2 | GLU | A | 225 | 31.281 | 48.958 | 26.368 | 1.00 | 40.78 | O |
| ATOM | 1707 | N | CYS | A | 226 | 25.539 | 45.258 | 26.836 | 1.00 | 21.15 | N |
| ATOM | 1708 | CA | CYS | A | 226 | 24.081 | 45.396 | 26.851 | 1.00 | 21.01 | C |
| ATOM | 1709 | C | CYS | A | 226 | 23.359 | 44.417 | 27.768 | 1.00 | 20.67 | C |
| ATOM | 1710 | O | CYS | A | 226 | 22.159 | 44.601 | 28.043 | 1.00 | 18.85 | O |
| ATOM | 1711 | CB | CYS | A | 226 | 23.520 | 45.190 | 25.447 | 1.00 | 20.88 | C |
| ATOM | 1712 | SG | CYS | A | 226 | 24.194 | 46.296 | 24.190 | 1.00 | 22.39 | S |
| ATOM | 1713 | N | LEU | A | 227 | 24.085 | 43.399 | 28.256 | 1.00 | 20.56 | N |
| ATOM | 1714 | CA | LEU | A | 227 | 23.461 | 42.304 | 28.985 | 1.00 | 20.48 | C |
| ATOM | 1715 | C | LEU | A | 227 | 23.795 | 42.185 | 30.466 | 1.00 | 20.42 | C |
| ATOM | 1716 | O | LEU | A | 227 | 23.180 | 41.398 | 31.187 | 1.00 | 20.78 | O |
| ATOM | 1717 | CB | LEU | A | 227 | 23.737 | 41.003 | 28.232 | 1.00 | 21.20 | C |
| ATOM | 1718 | CG | LEU | A | 227 | 22.865 | 40.993 | 26.963 | 1.00 | 22.96 | C |
| ATOM | 1719 | CD1 | LEU | A | 227 | 23.373 | 40.023 | 25.929 | 1.00 | 24.99 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1720 | CD2 | LEU | A | 227 | 21.420 | 40.655 | 27.323 | 1.00 | 24.79 | C |
| ATOM | 1721 | N | TYR | A | 228 | 24.793 | 42.939 | 30.901 | 1.00 | 20.08 | N |
| ATOM | 1722 | CA | TYR | A | 228 | 25.060 | 43.127 | 32.303 | 1.00 | 19.66 | C |
| ATOM | 1723 | C | TYR | A | 228 | 25.061 | 41.858 | 33.165 | 1.00 | 19.95 | C |
| ATOM | 1724 | O | TYR | A | 228 | 24.229 | 41.697 | 34.058 | 1.00 | 19.69 | O |
| ATOM | 1725 | CB | TYR | A | 228 | 24.050 | 44.137 | 32.857 | 1.00 | 19.77 | C |
| ATOM | 1726 | CG | TYR | A | 228 | 24.028 | 45.481 | 32.119 | 1.00 | 19.37 | C |
| ATOM | 1727 | CD1 | TYR | A | 228 | 24.836 | 46.513 | 32.515 | 1.00 | 18.65 | C |
| ATOM | 1728 | CD2 | TYR | A | 228 | 23.180 | 45.697 | 31.036 | 1.00 | 19.82 | C |
| ATOM | 1729 | CE1 | TYR | A | 228 | 24.819 | 47.759 | 31.862 | 1.00 | 20.56 | C |
| ATOM | 1730 | CE2 | TYR | A | 228 | 23.143 | 46.920 | 30.380 | 1.00 | 20.78 | C |
| ATOM | 1731 | CZ | TYR | A | 228 | 23.962 | 47.956 | 30.801 | 1.00 | 20.88 | C |
| ATOM | 1732 | OH | TYR | A | 228 | 23.944 | 49.174 | 30.152 | 1.00 | 19.73 | O |
| ATOM | 1733 | N | PRO | A | 229 | 26.028 | 40.981 | 32.941 | 1.00 | 19.99 | N |
| ATOM | 1734 | CA | PRO | A | 229 | 26.140 | 39.781 | 33.768 | 1.00 | 20.44 | C |
| ATOM | 1735 | C | PRO | A | 229 | 26.481 | 40.141 | 35.196 | 1.00 | 19.99 | C |
| ATOM | 1736 | O | PRO | A | 229 | 27.130 | 41.166 | 35.451 | 1.00 | 20.03 | O |
| ATOM | 1737 | CB | PRO | A | 229 | 27.334 | 39.043 | 33.157 | 1.00 | 20.11 | C |
| ATOM | 1738 | CG | PRO | A | 229 | 28.125 | 40.130 | 32.541 | 1.00 | 21.04 | C |
| ATOM | 1739 | CD | PRO | A | 229 | 27.099 | 41.050 | 31.935 | 1.00 | 19.79 | C |
| ATOM | 1740 | N | TYR | A | 230 | 26.044 | 39.294 | 36.115 | 1.00 | 19.50 | N |
| ATOM | 1741 | CA | TYR | A | 230 | 26.348 | 39.458 | 37.511 | 1.00 | 19.17 | C |
| ATOM | 1742 | C | TYR | A | 230 | 27.860 | 39.464 | 37.704 | 1.00 | 19.14 | C |
| ATOM | 1743 | O | TYR | A | 230 | 28.598 | 39.060 | 36.832 | 1.00 | 18.83 | O |
| ATOM | 1744 | CB | TYR | A | 230 | 25.746 | 38.313 | 38.320 | 1.00 | 18.51 | C |
| ATOM | 1745 | CG | TYR | A | 230 | 24.253 | 38.411 | 38.531 | 1.00 | 18.95 | C |
| ATOM | 1746 | CD1 | TYR | A | 230 | 23.368 | 37.949 | 37.560 | 1.00 | 18.39 | C |
| ATOM | 1747 | CD2 | TYR | A | 230 | 23.719 | 38.969 | 39.707 | 1.00 | 18.65 | C |
| ATOM | 1748 | CE1 | TYR | A | 230 | 22.001 | 38.006 | 37.751 | 1.00 | 17.34 | C |
| ATOM | 1749 | CE2 | TYR | A | 230 | 22.337 | 39.043 | 39.903 | 1.00 | 17.05 | C |
| ATOM | 1750 | CZ | TYR | A | 230 | 21.492 | 38.550 | 38.909 | 1.00 | 17.79 | C |
| ATOM | 1751 | OH | TYR | A | 230 | 20.127 | 38.601 | 39.051 | 1.00 | 19.77 | O |
| ATOM | 1752 | N | PRO | A | 231 | 28.316 | 39.963 | 38.843 | 1.00 | 19.95 | N |
| ATOM | 1753 | CA | PRO | A | 231 | 29.722 | 39.829 | 39.213 | 1.00 | 20.42 | C |
| ATOM | 1754 | C | PRO | A | 231 | 30.157 | 38.339 | 39.187 | 1.00 | 20.93 | C |
| ATOM | 1755 | O | PRO | A | 231 | 29.345 | 37.463 | 39.506 | 1.00 | 20.71 | O |
| ATOM | 1756 | CB | PRO | A | 231 | 29.755 | 40.369 | 40.642 | 1.00 | 20.70 | C |
| ATOM | 1757 | CG | PRO | A | 231 | 28.588 | 41.341 | 40.716 | 1.00 | 20.76 | C |
| ATOM | 1758 | CD | PRO | A | 231 | 27.528 | 40.701 | 39.845 | 1.00 | 19.53 | C |
| ATOM | 1759 | N | VAL | A | 232 | 31.413 | 38.067 | 38.831 | 1.00 | 20.93 | N |
| ATOM | 1760 | CA | VAL | A | 232 | 31.906 | 36.685 | 38.742 | 1.00 | 21.31 | C |
| ATOM | 1761 | C | VAL | A | 232 | 31.722 | 35.843 | 40.014 | 1.00 | 20.95 | C |
| ATOM | 1762 | O | VAL | A | 232 | 31.431 | 34.650 | 39.934 | 1.00 | 20.50 | O |
| ATOM | 1763 | CB | VAL | A | 232 | 33.398 | 36.655 | 38.304 | 1.00 | 21.35 | C |
| ATOM | 1764 | CG1 | VAL | A | 232 | 34.029 | 35.280 | 38.552 | 1.00 | 22.23 | C |
| ATOM | 1765 | CG2 | VAL | A | 232 | 33.533 | 37.031 | 36.850 | 1.00 | 21.71 | C |
| ATOM | 1766 | N | HIS | A | 233 | 31.872 | 36.455 | 41.181 | 1.00 | 21.10 | N |
| ATOM | 1767 | CA | HIS | A | 233 | 31.742 | 35.721 | 42.438 | 1.00 | 21.01 | C |
| ATOM | 1768 | C | HIS | A | 233 | 30.302 | 35.571 | 42.944 | 1.00 | 20.95 | C |
| ATOM | 1769 | O | HIS | A | 233 | 30.045 | 34.864 | 43.914 | 1.00 | 19.92 | O |
| ATOM | 1770 | CB | HIS | A | 233 | 32.606 | 36.363 | 43.501 | 1.00 | 21.12 | C |
| ATOM | 1771 | CG | HIS | A | 233 | 34.063 | 36.342 | 43.174 | 1.00 | 21.52 | C |
| ATOM | 1772 | ND1 | HIS | A | 233 | 34.720 | 37.424 | 42.625 | 1.00 | 22.78 | N |
| ATOM | 1773 | CD2 | HIS | A | 233 | 34.993 | 35.368 | 43.318 | 1.00 | 22.27 | C |
| ATOM | 1774 | CE1 | HIS | A | 233 | 35.994 | 37.114 | 42.446 | 1.00 | 24.00 | C |
| ATOM | 1775 | NE2 | HIS | A | 233 | 36.186 | 35.870 | 42.857 | 1.00 | 23.34 | N |
| ATOM | 1776 | N | HIS | A | 234 | 29.364 | 36.236 | 42.288 | 1.00 | 20.94 | N |
| ATOM | 1777 | CA | HIS | A | 234 | 27.959 | 36.081 | 42.630 | 1.00 | 21.27 | C |
| ATOM | 1778 | C | HIS | A | 234 | 27.493 | 34.722 | 42.103 | 1.00 | 21.28 | C |
| ATOM | 1779 | O | HIS | A | 234 | 28.022 | 34.233 | 41.107 | 1.00 | 21.02 | O |
| ATOM | 1780 | CB | HIS | A | 234 | 27.169 | 37.203 | 41.989 | 1.00 | 21.52 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1781 | CG | HIS | A | 234 | 25.730 | 37.253 | 42.374 | 1.00 | 21.54 | C |
| ATOM | 1782 | ND1 | HIS | A | 234 | 24.769 | 36.498 | 41.740 | 1.00 | 21.95 | N |
| ATOM | 1783 | CD2 | HIS | A | 234 | 25.073 | 38.028 | 43.269 | 1.00 | 22.67 | C |
| ATOM | 1784 | CE1 | HIS | A | 234 | 23.585 | 36.779 | 42.254 | 1.00 | 22.38 | C |
| ATOM | 1785 | NE2 | HIS | A | 234 | 23.743 | 37.700 | 43.187 | 1.00 | 21.91 | N |
| ATOM | 1786 | N | PRO | A | 235 | 26.551 | 34.087 | 42.792 | 1.00 | 21.11 | N |
| ATOM | 1787 | CA | PRO | A | 235 | 25.999 | 32.809 | 42.338 | 1.00 | 21.46 | C |
| ATOM | 1788 | C | PRO | A | 235 | 25.461 | 32.835 | 40.916 | 1.00 | 21.10 | C |
| ATOM | 1789 | O | PRO | A | 235 | 25.517 | 31.802 | 40.244 | 1.00 | 20.37 | O |
| ATOM | 1790 | CB | PRO | A | 235 | 24.860 | 32.551 | 43.325 | 1.00 | 21.90 | C |
| ATOM | 1791 | CG | PRO | A | 235 | 25.316 | 33.240 | 44.574 | 1.00 | 22.00 | C |
| ATOM | 1792 | CD | PRO | A | 235 | 26.007 | 34.485 | 44.100 | 1.00 | 21.41 | C |
| ATOM | 1793 | N | CYS | A | 236 | 24.997 | 33.989 | 40.452 | 1.00 | 20.41 | N |
| ATOM | 1794 | CA | CYS | A | 236 | 24.456 | 34.077 | 39.110 | 1.00 | 20.17 | C |
| ATOM | 1795 | C | CYS | A | 236 | 25.503 | 34.554 | 38.107 | 1.00 | 20.00 | C |
| ATOM | 1796 | O | CYS | A | 236 | 25.180 | 35.111 | 37.061 | 1.00 | 20.30 | O |
| ATOM | 1797 | CB | CYS | A | 236 | 23.195 | 34.924 | 39.090 | 1.00 | 19.66 | C |
| ATOM | 1798 | SG | CYS | A | 236 | 21.914 | 34.209 | 40.133 | 1.00 | 20.71 | S |
| ATOM | 1799 | N | ASP | A | 237 | 26.768 | 34.311 | 38.433 | 1.00 | 19.87 | N |
| ATOM | 1800 | CA | ASP | A | 237 | 27.857 | 34.498 | 37.485 | 1.00 | 19.60 | C |
| ATOM | 1801 | C | ASP | A | 237 | 27.459 | 33.915 | 36.105 | 1.00 | 19.48 | C |
| ATOM | 1802 | O | ASP | A | 237 | 26.883 | 32.834 | 36.020 | 1.00 | 18.94 | O |
| ATOM | 1803 | CB | ASP | A | 237 | 29.075 | 33.789 | 38.031 | 1.00 | 19.20 | C |
| ATOM | 1804 | CG | ASP | A | 237 | 30.268 | 33.842 | 37.107 | 1.00 | 20.58 | C |
| ATOM | 1805 | OD1 | ASP | A | 237 | 30.477 | 34.871 | 36.373 | 1.00 | 18.56 | O |
| ATOM | 1806 | OD2 | ASP | A | 237 | 31.070 | 32.868 | 37.077 | 1.00 | 19.51 | O |
| ATOM | 1807 | N | ARG | A | 238 | 27.749 | 34.675 | 35.056 | 1.00 | 19.85 | N |
| ATOM | 1808 | CA | ARG | A | 238 | 27.459 | 34.332 | 33.664 | 1.00 | 20.90 | C |
| ATOM | 1809 | C | ARG | A | 238 | 26.002 | 34.572 | 33.247 | 1.00 | 20.67 | C |
| ATOM | 1810 | O | ARG | A | 238 | 25.709 | 34.491 | 32.059 | 1.00 | 21.20 | O |
| ATOM | 1811 | CB | ARG | A | 238 | 27.854 | 32.876 | 33.319 | 1.00 | 21.44 | C |
| ATOM | 1812 | CG | ARG | A | 238 | 29.330 | 32.585 | 33.482 | 1.00 | 21.04 | C |
| ATOM | 1813 | CD | ARG | A | 238 | 29.710 | 31.150 | 33.145 | 1.00 | 22.38 | C |
| ATOM | 1814 | NE | ARG | A | 238 | 29.080 | 30.243 | 34.085 | 1.00 | 23.86 | N |
| ATOM | 1815 | CZ | ARG | A | 238 | 27.937 | 29.584 | 33.874 | 1.00 | 25.81 | C |
| ATOM | 1816 | NH1 | ARG | A | 238 | 27.262 | 29.686 | 32.712 | 1.00 | 24.18 | N |
| ATOM | 1817 | NH2 | ARG | A | 238 | 27.471 | 28.810 | 34.849 | 1.00 | 27.18 | N |
| ATOM | 1818 | N | GLN | A | 239 | 25.105 | 34.845 | 34.190 | 1.00 | 19.94 | N |
| ATOM | 1819 | CA | GLN | A | 239 | 23.722 | 35.141 | 33.833 | 1.00 | 20.58 | C |
| ATOM | 1820 | C | GLN | A | 239 | 23.535 | 36.661 | 33.740 | 1.00 | 20.50 | C |
| ATOM | 1821 | O | GLN | A | 239 | 24.219 | 37.402 | 34.446 | 1.00 | 20.63 | O |
| ATOM | 1822 | CB | GLN | A | 239 | 22.735 | 34.591 | 34.863 | 1.00 | 20.32 | C |
| ATOM | 1823 | CG | GLN | A | 239 | 23.159 | 33.314 | 35.594 | 1.00 | 20.84 | C |
| ATOM | 1824 | CD | GLN | A | 239 | 23.367 | 32.137 | 34.673 | 1.00 | 21.23 | C |
| ATOM | 1825 | OE1 | GLN | A | 239 | 22.434 | 31.675 | 34.014 | 1.00 | 21.22 | O |
| ATOM | 1826 | NE2 | GLN | A | 239 | 24.591 | 31.655 | 34.616 | 1.00 | 20.93 | N |
| ATOM | 1827 | N | SER | A | 240 | 22.600 | 37.112 | 32.900 | 1.00 | 20.07 | N |
| ATOM | 1828 | CA | SER | A | 240 | 22.282 | 38.533 | 32.768 | 1.00 | 20.18 | C |
| ATOM | 1829 | C | SER | A | 240 | 21.498 | 39.027 | 33.969 | 1.00 | 20.71 | C |
| ATOM | 1830 | O | SER | A | 240 | 20.619 | 38.316 | 34.467 | 1.00 | 20.85 | O |
| ATOM | 1831 | CB | SER | A | 240 | 21.405 | 38.776 | 31.539 | 1.00 | 20.29 | C |
| ATOM | 1832 | OG | SER | A | 240 | 21.007 | 40.137 | 31.454 | 1.00 | 21.43 | O |
| ATOM | 1833 | N | GLN | A | 241 | 21.793 | 40.246 | 34.426 | 1.00 | 20.46 | N |
| ATOM | 1834 | CA | GLN | A | 241 | 21.013 | 40.839 | 35.496 | 1.00 | 20.42 | C |
| ATOM | 1835 | C | GLN | A | 241 | 19.711 | 41.433 | 34.965 | 1.00 | 20.26 | C |
| ATOM | 1836 | O | GLN | A | 241 | 18.839 | 41.767 | 35.726 | 1.00 | 19.62 | O |
| ATOM | 1837 | CB | GLN | A | 241 | 21.770 | 41.949 | 36.201 | 1.00 | 20.32 | C |
| ATOM | 1838 | CG | GLN | A | 241 | 23.019 | 41.544 | 36.912 | 1.00 | 20.58 | C |
| ATOM | 1839 | CD | GLN | A | 241 | 23.771 | 42.767 | 37.423 | 1.00 | 21.94 | C |
| ATOM | 1840 | OE1 | GLN | A | 241 | 23.524 | 43.210 | 38.514 | 1.00 | 23.52 | O |
| ATOM | 1841 | NE2 | GLN | A | 241 | 24.670 | 43.304 | 36.624 | 1.00 | 20.84 | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1842 | N | VAL | A | 242 | 19.557 | 41.563 | 33.659 | 1.00 | 20.57 | N |
| ATOM | 1843 | CA | VAL | A | 242 | 18.361 | 42.229 | 33.182 | 1.00 | 20.73 | C |
| ATOM | 1844 | C | VAL | A | 242 | 17.173 | 41.309 | 33.246 | 1.00 | 20.69 | C |
| ATOM | 1845 | O | VAL | A | 242 | 17.244 | 40.190 | 32.757 | 1.00 | 21.13 | O |
| ATOM | 1846 | CB | VAL | A | 242 | 18.498 | 42.667 | 31.712 | 1.00 | 21.03 | C |
| ATOM | 1847 | CG1 | VAL | A | 242 | 17.204 | 43.377 | 31.250 | 1.00 | 20.85 | C |
| ATOM | 1848 | CG2 | VAL | A | 242 | 19.723 | 43.527 | 31.498 | 1.00 | 20.71 | C |
| ATOM | 1849 | N | ASP | A | 243 | 16.071 | 41.786 | 33.813 | 1.00 | 20.62 | N |
| ATOM | 1850 | CA | ASP | A | 243 | 14.807 | 41.042 | 33.788 | 1.00 | 20.64 | C |
| ATOM | 1851 | C | ASP | A | 243 | 14.148 | 41.348 | 32.448 | 1.00 | 20.94 | C |
| ATOM | 1852 | O | ASP | A | 243 | 13.591 | 42.438 | 32.230 | 1.00 | 19.75 | O |
| ATOM | 1853 | CB | ASP | A | 243 | 13.916 | 41.471 | 34.963 | 1.00 | 20.88 | C |
| ATOM | 1854 | CG | ASP | A | 243 | 12.526 | 40.894 | 34.898 | 1.00 | 21.39 | C |
| ATOM | 1855 | OD1 | ASP | A | 243 | 12.209 | 40.153 | 33.941 | 1.00 | 23.25 | O |
| ATOM | 1856 | OD2 | ASP | A | 243 | 11.672 | 41.130 | 35.784 | 1.00 | 23.49 | O |
| ATOM | 1857 | N | PHE | A | 244 | 14.238 | 40.385 | 31.541 | 1.00 | 21.19 | N |
| ATOM | 1858 | CA | PHE | A | 244 | 13.717 | 40.549 | 30.197 | 1.00 | 21.56 | C |
| ATOM | 1859 | C | PHE | A | 244 | 12.225 | 40.916 | 30.204 | 1.00 | 22.49 | C |
| ATOM | 1860 | O | PHE | A | 244 | 11.734 | 41.521 | 29.260 | 1.00 | 21.85 | O |
| ATOM | 1861 | CB | PHE | A | 244 | 13.940 | 39.275 | 29.378 | 1.00 | 21.85 | C |
| ATOM | 1862 | CG | PHE | A | 244 | 15.316 | 39.152 | 28.743 | 1.00 | 20.87 | C |
| ATOM | 1863 | CD1 | PHE | A | 244 | 16.457 | 39.540 | 29.399 | 1.00 | 20.74 | C |
| ATOM | 1864 | CD2 | PHE | A | 244 | 15.446 | 38.617 | 27.483 | 1.00 | 21.00 | C |
| ATOM | 1865 | CE1 | PHE | A | 244 | 17.691 | 39.407 | 28.810 | 1.00 | 19.77 | C |
| ATOM | 1866 | CE2 | PHE | A | 244 | 16.687 | 38.470 | 26.890 | 1.00 | 20.94 | C |
| ATOM | 1867 | CZ | PHE | A | 244 | 17.805 | 38.881 | 27.551 | 1.00 | 20.34 | C |
| ATOM | 1868 | N | ASP | A | 245 | 11.500 | 40.554 | 31.259 | 1.00 | 23.56 | N |
| ATOM | 1869 | CA | ASP | A | 245 | 10.072 | 40.831 | 31.311 | 1.00 | 24.26 | C |
| ATOM | 1870 | C | ASP | A | 245 | 9.794 | 42.256 | 31.814 | 1.00 | 24.66 | C |
| ATOM | 1871 | O | ASP | A | 245 | 8.711 | 42.762 | 31.607 | 1.00 | 24.21 | O |
| ATOM | 1872 | CB | ASP | A | 245 | 9.353 | 39.841 | 32.222 | 1.00 | 24.74 | C |
| ATOM | 1873 | CG | ASP | A | 245 | 9.408 | 38.427 | 31.721 | 1.00 | 26.56 | C |
| ATOM | 1874 | OD1 | ASP | A | 245 | 9.368 | 38.210 | 30.493 | 1.00 | 28.81 | O |
| ATOM | 1875 | OD2 | ASP | A | 245 | 9.489 | 37.455 | 32.498 | 1.00 | 28.39 | O |
| ATOM | 1876 | N | ASN | A | 246 | 10.758 | 42.876 | 32.492 | 1.00 | 24.80 | N |
| ATOM | 1877 | CA | ASN | A | 246 | 10.605 | 44.244 | 32.989 | 1.00 | 25.56 | C |
| ATOM | 1878 | C | ASN | A | 246 | 11.960 | 44.902 | 33.106 | 1.00 | 25.31 | C |
| ATOM | 1879 | O | ASN | A | 246 | 12.500 | 45.064 | 34.205 | 1.00 | 25.43 | O |
| ATOM | 1880 | CB | ASN | A | 246 | 9.912 | 44.285 | 34.345 | 1.00 | 26.09 | C |
| ATOM | 1881 | CG | ASN | A | 246 | 9.555 | 45.716 | 34.765 | 1.00 | 29.59 | C |
| ATOM | 1882 | OD1 | ASN | A | 246 | 9.366 | 46.598 | 33.912 | 1.00 | 32.67 | O |
| ATOM | 1883 | ND2 | ASN | A | 246 | 9.468 | 45.954 | 36.075 | 1.00 | 33.42 | N |
| ATOM | 1884 | N | PRO | A | 247 | 12.525 | 45.257 | 31.961 | 1.00 | 25.08 | N |
| ATOM | 1885 | CA | PRO | A | 247 | 13.885 | 45.782 | 31.911 | 1.00 | 24.89 | C |
| ATOM | 1886 | C | PRO | A | 247 | 13.992 | 47.144 | 32.579 | 1.00 | 24.95 | C |
| ATOM | 1887 | O | PRO | A | 247 | 13.217 | 48.049 | 32.297 | 1.00 | 24.55 | O |
| ATOM | 1888 | CB | PRO | A | 247 | 14.182 | 45.899 | 30.413 | 1.00 | 25.05 | C |
| ATOM | 1889 | CG | PRO | A | 247 | 13.016 | 45.325 | 29.702 | 1.00 | 25.39 | C |
| ATOM | 1890 | CD | PRO | A | 247 | 11.890 | 45.184 | 30.640 | 1.00 | 25.02 | C |
| ATOM | 1891 | N | ASP | A | 248 | 14.976 | 47.267 | 33.460 | 1.00 | 24.53 | N |
| ATOM | 1892 | CA | ASP | A | 248 | 15.216 | 48.489 | 34.167 | 1.00 | 24.65 | C |
| ATOM | 1893 | C | ASP | A | 248 | 16.271 | 49.284 | 33.389 | 1.00 | 24.54 | C |
| ATOM | 1894 | O | ASP | A | 248 | 17.472 | 49.077 | 33.552 | 1.00 | 23.15 | O |
| ATOM | 1895 | CB | ASP | A | 248 | 15.706 | 48.144 | 35.564 | 1.00 | 24.64 | C |
| ATOM | 1896 | CG | ASP | A | 248 | 15.787 | 49.343 | 36.454 | 1.00 | 26.02 | C |
| ATOM | 1897 | OD1 | ASP | A | 248 | 16.035 | 50.466 | 35.944 | 1.00 | 26.95 | O |
| ATOM | 1898 | OD2 | ASP | A | 248 | 15.609 | 49.249 | 37.684 | 1.00 | 27.69 | O |
| ATOM | 1899 | N | TYR | A | 249 | 15.812 | 50.181 | 32.525 | 1.00 | 24.81 | N |
| ATOM | 1900 | CA | TYR | A | 249 | 16.720 | 50.936 | 31.673 | 1.00 | 25.45 | C |
| ATOM | 1901 | C | TYR | A | 249 | 17.573 | 51.954 | 32.426 | 1.00 | 25.90 | C |
| ATOM | 1902 | O | TYR | A | 249 | 18.585 | 52.421 | 31.897 | 1.00 | 25.80 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1903 | CB | TYR | A | 249 | 15.948 | 51.615 | 30.544 | 1.00 | 25.57 | C |
| ATOM | 1904 | CG | TYR | A | 249 | 15.244 | 50.651 | 29.630 | 1.00 | 24.58 | C |
| ATOM | 1905 | CD1 | TYR | A | 249 | 15.930 | 49.624 | 29.003 | 1.00 | 25.44 | C |
| ATOM | 1906 | CD2 | TYR | A | 249 | 13.890 | 50.764 | 29.404 | 1.00 | 24.48 | C |
| ATOM | 1907 | CE1 | TYR | A | 249 | 15.276 | 48.731 | 28.173 | 1.00 | 25.01 | C |
| ATOM | 1908 | CE2 | TYR | A | 249 | 13.234 | 49.892 | 28.583 | 1.00 | 24.43 | C |
| ATOM | 1909 | CZ | TYR | A | 249 | 13.927 | 48.883 | 27.969 | 1.00 | 24.47 | C |
| ATOM | 1910 | OH | TYR | A | 249 | 13.252 | 48.043 | 27.142 | 1.00 | 25.97 | O |
| ATOM | 1911 | N | GLU | A | 250 | 17.195 | 52.278 | 33.660 | 1.00 | 26.10 | N |
| ATOM | 1912 | CA | GLU | A | 250 | 17.999 | 53.190 | 34.458 | 1.00 | 26.93 | C |
| ATOM | 1913 | C | GLU | A | 250 | 19.259 | 52.492 | 34.929 | 1.00 | 25.85 | C |
| ATOM | 1914 | O | GLU | A | 250 | 20.329 | 53.086 | 34.964 | 1.00 | 25.90 | O |
| ATOM | 1915 | CB | GLU | A | 250 | 17.219 | 53.740 | 35.661 | 1.00 | 27.56 | C |
| ATOM | 1916 | CG | GLU | A | 250 | 16.021 | 54.576 | 35.246 | 1.00 | 32.34 | C |
| ATOM | 1917 | CD | GLU | A | 250 | 15.420 | 55.366 | 36.385 | 1.00 | 36.85 | C |
| ATOM | 1918 | OE1 | GLU | A | 250 | 15.945 | 55.309 | 37.516 | 1.00 | 42.35 | O |
| ATOM | 1919 | OE2 | GLU | A | 250 | 14.422 | 56.057 | 36.142 | 1.00 | 40.82 | O |
| ATOM | 1920 | N | ARG | A | 251 | 19.136 | 51.233 | 35.315 | 1.00 | 24.58 | N |
| ATOM | 1921 | CA | ARG | A | 251 | 20.297 | 50.502 | 35.756 | 1.00 | 23.76 | C |
| ATOM | 1922 | C | ARG | A | 251 | 21.030 | 49.909 | 34.568 | 1.00 | 22.91 | C |
| ATOM | 1923 | O | ARG | A | 251 | 22.242 | 49.773 | 34.602 | 1.00 | 22.42 | O |
| ATOM | 1924 | CB | ARG | A | 251 | 19.896 | 49.374 | 36.696 | 1.00 | 24.55 | C |
| ATOM | 1925 | CG | ARG | A | 251 | 19.421 | 49.802 | 38.077 | 1.00 | 25.88 | C |
| ATOM | 1926 | CD | ARG | A | 251 | 18.894 | 48.629 | 38.921 | 1.00 | 29.50 | C |
| ATOM | 1927 | NE | ARG | A | 251 | 19.993 | 47.764 | 39.349 | 1.00 | 31.63 | N |
| ATOM | 1928 | CZ | ARG | A | 251 | 19.894 | 46.467 | 39.623 | 1.00 | 33.13 | C |
| ATOM | 1929 | NH1 | ARG | A | 251 | 18.736 | 45.826 | 39.521 | 1.00 | 33.12 | N |
| ATOM | 1930 | NH2 | ARG | A | 251 | 20.978 | 45.805 | 39.998 | 1.00 | 33.93 | N |
| ATOM | 1931 | N | PHE | A | 252 | 20.300 | 49.560 | 33.515 | 1.00 | 21.47 | N |
| ATOM | 1932 | CA | PHE | A | 252 | 20.898 | 48.863 | 32.379 | 1.00 | 21.32 | C |
| ATOM | 1933 | C | PHE | A | 252 | 20.576 | 49.552 | 31.056 | 1.00 | 20.68 | C |
| ATOM | 1934 | O | PHE | A | 252 | 19.934 | 48.984 | 30.187 | 1.00 | 20.79 | O |
| ATOM | 1935 | CB | PHE | A | 252 | 20.355 | 47.434 | 32.344 | 1.00 | 21.09 | C |
| ATOM | 1936 | CG | PHE | A | 252 | 20.373 | 46.738 | 33.690 | 1.00 | 20.96 | C |
| ATOM | 1937 | CD1 | PHE | A | 252 | 21.555 | 46.560 | 34.376 | 1.00 | 19.28 | C |
| ATOM | 1938 | CD2 | PHE | A | 252 | 19.207 | 46.238 | 34.247 | 1.00 | 21.43 | C |
| ATOM | 1939 | CE1 | PHE | A | 252 | 21.571 | 45.891 | 35.609 | 1.00 | 20.54 | C |
| ATOM | 1940 | CE2 | PHE | A | 252 | 19.217 | 45.588 | 35.488 | 1.00 | 22.13 | C |
| ATOM | 1941 | CZ | PHE | A | 252 | 20.403 | 45.414 | 36.156 | 1.00 | 20.96 | C |
| ATOM | 1942 | N | PRO | A | 253 | 21.057 | 50.767 | 30.884 | 1.00 | 20.56 | N |
| ATOM | 1943 | CA | PRO | A | 253 | 20.658 | 51.566 | 29.714 | 1.00 | 20.38 | C |
| ATOM | 1944 | C | PRO | A | 253 | 20.984 | 50.916 | 28.361 | 1.00 | 20.20 | C |
| ATOM | 1945 | O | PRO | A | 253 | 20.191 | 51.053 | 27.428 | 1.00 | 19.48 | O |
| ATOM | 1946 | CB | PRO | A | 253 | 21.383 | 52.903 | 29.928 | 1.00 | 19.77 | C |
| ATOM | 1947 | CG | PRO | A | 253 | 22.562 | 52.555 | 30.895 | 1.00 | 20.60 | C |
| ATOM | 1948 | CD | PRO | A | 253 | 21.986 | 51.484 | 31.782 | 1.00 | 20.69 | C |
| ATOM | 1949 | N | ASN | A | 254 | 22.091 | 50.187 | 28.240 | 1.00 | 20.32 | N |
| ATOM | 1950 | CA | ASN | A | 254 | 22.409 | 49.613 | 26.938 | 1.00 | 20.12 | C |
| ATOM | 1951 | C | ASN | A | 254 | 21.572 | 48.393 | 26.554 | 1.00 | 19.96 | C |
| ATOM | 1952 | O | ASN | A | 254 | 21.675 | 47.892 | 25.441 | 1.00 | 19.16 | O |
| ATOM | 1953 | CB | ASN | A | 254 | 23.893 | 49.336 | 26.784 | 1.00 | 20.06 | C |
| ATOM | 1954 | CG | ASN | A | 254 | 24.706 | 50.601 | 26.697 | 1.00 | 21.51 | C |
| ATOM | 1955 | OD1 | ASN | A | 254 | 25.502 | 50.896 | 27.598 | 1.00 | 23.96 | O |
| ATOM | 1956 | ND2 | ASN | A | 254 | 24.514 | 51.373 | 25.614 | 1.00 | 20.38 | N |
| ATOM | 1957 | N | PHE | A | 255 | 20.724 | 47.922 | 27.455 | 1.00 | 19.81 | N |
| ATOM | 1958 | CA | PHE | A | 255 | 19.807 | 46.858 | 27.063 | 1.00 | 19.54 | C |
| ATOM | 1959 | C | PHE | A | 255 | 18.855 | 47.384 | 25.977 | 1.00 | 19.69 | C |
| ATOM | 1960 | O | PHE | A | 255 | 18.194 | 46.606 | 25.274 | 1.00 | 19.77 | O |
| ATOM | 1961 | CB | PHE | A | 255 | 19.023 | 46.330 | 28.252 | 1.00 | 19.22 | C |
| ATOM | 1962 | CG | PHE | A | 255 | 18.269 | 45.105 | 27.940 | 1.00 | 20.47 | C |
| ATOM | 1963 | CD1 | PHE | A | 255 | 18.928 | 43.922 | 27.736 | 1.00 | 20.23 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1964 | CD2 | PHE | A | 255 | 16.909 | 45.148 | 27.758 | 1.00 | 20.13 | C |
| ATOM | 1965 | CE1 | PHE | A | 255 | 18.243 | 42.786 | 27.416 | 1.00 | 21.65 | C |
| ATOM | 1966 | CE2 | PHE | A | 255 | 16.227 | 44.023 | 27.432 | 1.00 | 20.73 | C |
| ATOM | 1967 | CZ | PHE | A | 255 | 16.886 | 42.842 | 27.257 | 1.00 | 22.63 | C |
| ATOM | 1968 | N | GLN | A | 256 | 18.790 | 48.707 | 25.841 | 1.00 | 19.89 | N |
| ATOM | 1969 | CA | GLN | A | 256 | 17.969 | 49.345 | 24.794 | 1.00 | 20.24 | C |
| ATOM | 1970 | C | GLN | A | 256 | 18.595 | 49.160 | 23.403 | 1.00 | 19.74 | C |
| ATOM | 1971 | O | GLN | A | 256 | 17.969 | 49.443 | 22.384 | 1.00 | 19.92 | O |
| ATOM | 1972 | CB | GLN | A | 256 | 17.778 | 50.849 | 25.095 | 1.00 | 20.01 | C |
| ATOM | 1973 | CG | GLN | A | 256 | 16.736 | 51.095 | 26.197 | 1.00 | 21.20 | C |
| ATOM | 1974 | CD | GLN | A | 256 | 16.741 | 52.513 | 26.764 | 1.00 | 22.14 | C |
| ATOM | 1975 | OE1 | GLN | A | 256 | 15.711 | 53.195 | 26.741 | 1.00 | 23.01 | O |
| ATOM | 1976 | NE2 | GLN | A | 256 | 17.874 | 52.943 | 27.298 | 1.00 | 21.42 | N |
| ATOM | 1977 | N | ASN | A | 257 | 19.845 | 48.716 | 23.385 | 1.00 | 19.66 | N |
| ATOM | 1978 | CA | ASN | A | 257 | 20.580 | 48.485 | 22.155 | 1.00 | 20.07 | C |
| ATOM | 1979 | C | ASN | A | 257 | 20.757 | 47.005 | 21.811 | 1.00 | 20.73 | C |
| ATOM | 1980 | O | ASN | A | 257 | 21.416 | 46.694 | 20.823 | 1.00 | 20.96 | O |
| ATOM | 1981 | CB | ASN | A | 257 | 21.969 | 49.100 | 22.232 | 1.00 | 19.17 | C |
| ATOM | 1982 | CG | ASN | A | 257 | 21.941 | 50.550 | 22.635 | 1.00 | 20.82 | C |
| ATOM | 1983 | OD1 | ASN | A | 257 | 22.413 | 50.902 | 23.722 | 1.00 | 21.51 | O |
| ATOM | 1984 | ND2 | ASN | A | 257 | 21.396 | 51.407 | 21.763 | 1.00 | 16.92 | N |
| ATOM | 1985 | N | VAL | A | 258 | 20.190 | 46.098 | 22.596 | 1.00 | 21.59 | N |
| ATOM | 1986 | CA | VAL | A | 258 | 20.410 | 44.660 | 22.347 | 1.00 | 23.34 | C |
| ATOM | 1987 | C | VAL | A | 258 | 19.671 | 44.172 | 21.112 | 1.00 | 23.85 | C |
| ATOM | 1988 | O | VAL | A | 258 | 18.549 | 44.611 | 20.818 | 1.00 | 24.10 | O |
| ATOM | 1989 | CB | VAL | A | 258 | 20.015 | 43.806 | 23.573 | 1.00 | 23.68 | C |
| ATOM | 1990 | CG1 | VAL | A | 258 | 18.507 | 43.720 | 23.685 | 1.00 | 24.12 | C |
| ATOM | 1991 | CG2 | VAL | A | 258 | 20.570 | 42.436 | 23.445 | 1.00 | 28.30 | C |
| ATOM | 1992 | N | VAL | A | 259 | 20.314 | 43.286 | 20.360 | 1.00 | 24.47 | N |
| ATOM | 1993 | CA | VAL | A | 259 | 19.705 | 42.721 | 19.154 | 1.00 | 24.91 | C |
| ATOM | 1994 | C | VAL | A | 259 | 20.004 | 41.215 | 19.140 | 1.00 | 24.93 | C |
| ATOM | 1995 | O | VAL | A | 259 | 21.152 | 40.829 | 19.119 | 1.00 | 25.32 | O |
| ATOM | 1996 | CB | VAL | A | 259 | 20.281 | 43.362 | 17.895 | 1.00 | 24.88 | C |
| ATOM | 1997 | CG1 | VAL | A | 259 | 19.667 | 42.738 | 16.670 | 1.00 | 26.38 | C |
| ATOM | 1998 | CG2 | VAL | A | 259 | 20.051 | 44.869 | 17.909 | 1.00 | 24.83 | C |
| ATOM | 1999 | N | GLY | A | 260 | 18.974 | 40.381 | 19.186 | 1.00 | 25.06 | N |
| ATOM | 2000 | CA | GLY | A | 260 | 19.166 | 38.944 | 19.232 | 1.00 | 25.64 | C |
| ATOM | 2001 | C | GLY | A | 260 | 19.076 | 38.221 | 17.887 | 1.00 | 25.42 | C |
| ATOM | 2002 | O | GLY | A | 260 | 18.679 | 38.796 | 16.869 | 1.00 | 25.77 | O |
| ATOM | 2003 | N | TYR | A | 261 | 19.497 | 36.965 | 17.907 | 1.00 | 25.04 | N |
| ATOM | 2004 | CA | TYR | A | 261 | 19.380 | 36.049 | 16.792 | 1.00 | 25.30 | C |
| ATOM | 2005 | C | TYR | A | 261 | 18.428 | 34.973 | 17.328 | 1.00 | 24.63 | C |
| ATOM | 2006 | O | TYR | A | 261 | 18.676 | 34.417 | 18.392 | 1.00 | 24.77 | O |
| ATOM | 2007 | CB | TYR | A | 261 | 20.729 | 35.414 | 16.482 | 1.00 | 25.84 | C |
| ATOM | 2008 | CG | TYR | A | 261 | 21.750 | 36.315 | 15.825 | 1.00 | 28.57 | C |
| ATOM | 2009 | CD1 | TYR | A | 261 | 21.821 | 36.423 | 14.447 | 1.00 | 34.41 | C |
| ATOM | 2010 | CD2 | TYR | A | 261 | 22.631 | 37.049 | 16.574 | 1.00 | 29.87 | C |
| ATOM | 2011 | CE1 | TYR | A | 261 | 22.752 | 37.255 | 13.838 | 1.00 | 35.64 | C |
| ATOM | 2012 | CE2 | TYR | A | 261 | 23.576 | 37.852 | 15.986 | 1.00 | 32.26 | C |
| ATOM | 2013 | CZ | TYR | A | 261 | 23.644 | 37.949 | 14.623 | 1.00 | 34.92 | C |
| ATOM | 2014 | OH | TYR | A | 261 | 24.582 | 38.772 | 14.047 | 1.00 | 38.39 | O |
| ATOM | 2015 | N | GLU | A | 262 | 17.325 | 34.698 | 16.658 | 1.00 | 23.64 | N |
| ATOM | 2016 | CA | GLU | A | 262 | 16.376 | 33.758 | 17.244 | 1.00 | 24.03 | C |
| ATOM | 2017 | C | GLU | A | 262 | 15.933 | 32.660 | 16.306 | 1.00 | 23.15 | C |
| ATOM | 2018 | O | GLU | A | 262 | 16.063 | 32.766 | 15.078 | 1.00 | 22.51 | O |
| ATOM | 2019 | CB | GLU | A | 262 | 15.172 | 34.482 | 17.861 | 1.00 | 24.11 | C |
| ATOM | 2020 | CG | GLU | A | 262 | 13.899 | 34.502 | 17.057 | 1.00 | 26.35 | C |
| ATOM | 2021 | CD | GLU | A | 262 | 12.744 | 35.177 | 17.785 | 1.00 | 27.98 | C |
| ATOM | 2022 | OE1 | GLU | A | 262 | 12.743 | 36.415 | 17.872 | 1.00 | 27.19 | O |
| ATOM | 2023 | OE2 | GLU | A | 262 | 11.818 | 34.476 | 18.254 | 1.00 | 29.21 | O |
| ATOM | 2024 | N | THR | A | 263 | 15.455 | 31.587 | 16.917 | 1.00 | 22.58 | N |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2025 | CA | THR | A | 263 | 14.939 | 30.458 | 16.170 | 1.00 | 22.52 | C |
| ATOM | 2026 | C | THR | A | 263 | 14.047 | 29.617 | 17.076 | 1.00 | 22.48 | C |
| ATOM | 2027 | O | THR | A | 263 | 14.107 | 29.712 | 18.313 | 1.00 | 22.14 | O |
| ATOM | 2028 | CB | THR | A | 263 | 16.117 | 29.607 | 15.659 | 1.00 | 22.55 | C |
| ATOM | 2029 | OG1 | THR | A | 263 | 15.665 | 28.666 | 14.675 | 1.00 | 22.25 | O |
| ATOM | 2030 | CG2 | THR | A | 263 | 16.693 | 28.743 | 16.770 | 1.00 | 22.79 | C |
| ATOM | 2031 | N | VAL | A | 264 | 13.208 | 28.797 | 16.472 | 1.00 | 21.62 | N |
| ATOM | 2032 | CA | VAL | A | 264 | 12.453 | 27.860 | 17.263 | 1.00 | 22.45 | C |
| ATOM | 2033 | C | VAL | A | 264 | 12.871 | 26.474 | 16.837 | 1.00 | 22.76 | C |
| ATOM | 2034 | O | VAL | A | 264 | 12.779 | 26.134 | 15.673 | 1.00 | 22.77 | O |
| ATOM | 2035 | CB | VAL | A | 264 | 10.964 | 28.027 | 17.087 | 1.00 | 23.08 | C |
| ATOM | 2036 | CG1 | VAL | A | 264 | 10.234 | 26.805 | 17.643 | 1.00 | 23.67 | C |
| ATOM | 2037 | CG2 | VAL | A | 264 | 10.499 | 29.344 | 17.767 | 1.00 | 22.75 | C |
| ATOM | 2038 | N | VAL | A | 265 | 13.389 | 25.695 | 17.777 | 1.00 | 22.93 | N |
| ATOM | 2039 | CA | VAL | A | 265 | 13.779 | 24.329 | 17.458 | 1.00 | 23.08 | C |
| ATOM | 2040 | C | VAL | A | 265 | 12.738 | 23.317 | 17.886 | 1.00 | 22.86 | C |
| ATOM | 2041 | O | VAL | A | 265 | 12.105 | 23.473 | 18.932 | 1.00 | 23.06 | O |
| ATOM | 2042 | CB | VAL | A | 265 | 15.143 | 23.937 | 18.075 | 1.00 | 22.94 | C |
| ATOM | 2043 | CG1 | VAL | A | 265 | 16.243 | 24.745 | 17.404 | 1.00 | 23.66 | C |
| ATOM | 2044 | CG2 | VAL | A | 265 | 15.169 | 24.122 | 19.592 | 1.00 | 22.99 | C |
| ATOM | 2045 | N | GLY | A | 266 | 12.574 | 22.290 | 17.056 | 1.00 | 21.77 | N |
| ATOM | 2046 | CA | GLY | A | 266 | 11.683 | 21.178 | 17.355 | 1.00 | 21.98 | C |
| ATOM | 2047 | C | GLY | A | 266 | 12.376 | 19.826 | 17.263 | 1.00 | 20.97 | C |
| ATOM | 2048 | O | GLY | A | 266 | 13.562 | 19.757 | 16.999 | 1.00 | 20.63 | O |
| ATOM | 2049 | N | PRO | A | 267 | 11.643 | 18.737 | 17.461 | 1.00 | 21.23 | N |
| ATOM | 2050 | CA | PRO | A | 267 | 12.253 | 17.403 | 17.427 | 1.00 | 20.68 | C |
| ATOM | 2051 | C | PRO | A | 267 | 13.126 | 17.183 | 16.203 | 1.00 | 20.04 | C |
| ATOM | 2052 | O | PRO | A | 267 | 12.666 | 17.371 | 15.081 | 1.00 | 19.35 | O |
| ATOM | 2053 | CB | PRO | A | 267 | 11.039 | 16.463 | 17.379 | 1.00 | 21.29 | C |
| ATOM | 2054 | CG | PRO | A | 267 | 9.970 | 17.202 | 18.037 | 1.00 | 22.85 | C |
| ATOM | 2055 | CD | PRO | A | 267 | 10.188 | 18.676 | 17.710 | 1.00 | 21.61 | C |
| ATOM | 2056 | N | GLY | A | 268 | 14.376 | 16.787 | 16.411 | 1.00 | 20.31 | N |
| ATOM | 2057 | CA | GLY | A | 268 | 15.278 | 16.518 | 15.305 | 1.00 | 19.95 | C |
| ATOM | 2058 | C | GLY | A | 268 | 16.256 | 17.627 | 14.993 | 1.00 | 20.50 | C |
| ATOM | 2059 | O | GLY | A | 268 | 17.277 | 17.400 | 14.311 | 1.00 | 21.62 | O |
| ATOM | 2060 | N | ASP | A | 269 | 15.965 | 18.831 | 15.477 | 1.00 | 19.81 | N |
| ATOM | 2061 | CA | ASP | A | 269 | 16.818 | 19.977 | 15.217 | 1.00 | 19.75 | C |
| ATOM | 2062 | C | ASP | A | 269 | 17.970 | 20.003 | 16.215 | 1.00 | 19.67 | C |
| ATOM | 2063 | O | ASP | A | 269 | 17.811 | 19.625 | 17.377 | 1.00 | 18.76 | O |
| ATOM | 2064 | CB | ASP | A | 269 | 16.032 | 21.288 | 15.386 | 1.00 | 19.99 | C |
| ATOM | 2065 | CG | ASP | A | 269 | 14.916 | 21.464 | 14.374 | 1.00 | 20.91 | C |
| ATOM | 2066 | OD1 | ASP | A | 269 | 14.935 | 20.842 | 13.287 | 1.00 | 22.13 | O |
| ATOM | 2067 | OD2 | ASP | A | 269 | 13.987 | 22.259 | 14.576 | 1.00 | 23.27 | O |
| ATOM | 2068 | N | VAL | A | 270 | 19.116 | 20.481 | 15.746 | 1.00 | 19.56 | N |
| ATOM | 2069 | CA | VAL | A | 270 | 20.276 | 20.700 | 16.595 | 1.00 | 19.57 | C |
| ATOM | 2070 | C | VAL | A | 270 | 20.747 | 22.137 | 16.444 | 1.00 | 19.33 | C |
| ATOM | 2071 | O | VAL | A | 270 | 21.033 | 22.594 | 15.352 | 1.00 | 19.78 | O |
| ATOM | 2072 | CB | VAL | A | 270 | 21.404 | 19.776 | 16.215 | 1.00 | 19.55 | C |
| ATOM | 2073 | CG1 | VAL | A | 270 | 22.646 | 20.154 | 16.966 | 1.00 | 20.05 | C |
| ATOM | 2074 | CG2 | VAL | A | 270 | 21.001 | 18.342 | 16.535 | 1.00 | 19.44 | C |
| ATOM | 2075 | N | LEU | A | 271 | 20.786 | 22.870 | 17.539 | 1.00 | 19.33 | N |
| ATOM | 2076 | CA | LEU | A | 271 | 21.263 | 24.229 | 17.501 | 1.00 | 19.02 | C |
| ATOM | 2077 | C | LEU | A | 271 | 22.677 | 24.272 | 18.036 | 1.00 | 19.15 | C |
| ATOM | 2078 | O | LEU | A | 271 | 22.961 | 23.787 | 19.130 | 1.00 | 18.74 | O |
| ATOM | 2079 | CB | LEU | A | 271 | 20.376 | 25.120 | 18.331 | 1.00 | 19.93 | C |
| ATOM | 2080 | CG | LEU | A | 271 | 20.892 | 26.549 | 18.573 | 1.00 | 20.11 | C |
| ATOM | 2081 | CD1 | LEU | A | 271 | 21.011 | 27.358 | 17.296 | 1.00 | 19.41 | C |
| ATOM | 2082 | CD2 | LEU | A | 271 | 19.979 | 27.245 | 19.555 | 1.00 | 20.25 | C |
| ATOM | 2083 | N | TYR | A | 272 | 23.582 | 24.818 | 17.244 | 1.00 | 19.15 | N |
| ATOM | 2084 | CA | TYR | A | 272 | 24.924 | 25.051 | 17.718 | 1.00 | 19.70 | C |
| ATOM | 2085 | C | TYR | A | 272 | 24.914 | 26.360 | 18.483 | 1.00 | 19.63 | C |

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ATOM   2086  O   TYR A 272      24.646  27.395  17.897  1.00 20.44           O
ATOM   2087  CB  TYR A 272      25.908  25.172  16.547  1.00 19.86           C
ATOM   2088  CG  TYR A 272      27.293  25.654  16.962  1.00 21.59           C
ATOM   2089  CD1 TYR A 272      27.952  25.093  18.048  1.00 22.02           C
ATOM   2090  CD2 TYR A 272      27.936  26.668  16.278  1.00 20.87           C
ATOM   2091  CE1 TYR A 272      29.214  25.522  18.421  1.00 19.87           C
ATOM   2092  CE2 TYR A 272      29.200  27.098  16.649  1.00 20.88           C
ATOM   2093  CZ  TYR A 272      29.834  26.517  17.721  1.00 21.07           C
ATOM   2094  OH  TYR A 272      31.091  26.937  18.104  1.00 18.93           O
ATOM   2095  N   ILE A 273      25.210  26.308  19.776  1.00 19.80           N
ATOM   2096  CA  ILE A 273      25.342  27.500  20.598  1.00 20.12           C
ATOM   2097  C   ILE A 273      26.837  27.683  20.883  1.00 20.39           C
ATOM   2098  O   ILE A 273      27.393  27.000  21.760  1.00 19.88           O
ATOM   2099  CB  ILE A 273      24.576  27.366  21.901  1.00 19.72           C
ATOM   2100  CG1 ILE A 273      23.111  27.045  21.624  1.00 20.57           C
ATOM   2101  CG2 ILE A 273      24.661  28.695  22.696  1.00 20.99           C
ATOM   2102  CD1 ILE A 273      22.296  26.797  22.876  1.00 20.93           C
ATOM   2103  N   PRO A 274      27.487  28.611  20.182  1.00 20.23           N
ATOM   2104  CA  PRO A 274      28.938  28.743  20.326  1.00 21.16           C
ATOM   2105  C   PRO A 274      29.289  29.264  21.704  1.00 21.39           C
ATOM   2106  O   PRO A 274      28.520  30.027  22.317  1.00 20.89           O
ATOM   2107  CB  PRO A 274      29.353  29.757  19.230  1.00 21.62           C
ATOM   2108  CG  PRO A 274      28.089  30.056  18.410  1.00 21.22           C
ATOM   2109  CD  PRO A 274      26.919  29.621  19.282  1.00 20.51           C
ATOM   2110  N   MET A 275      30.450  28.831  22.180  1.00 21.53           N
ATOM   2111  CA  MET A 275      30.953  29.207  23.479  1.00 22.30           C
ATOM   2112  C   MET A 275      30.920  30.734  23.636  1.00 21.94           C
ATOM   2113  O   MET A 275      31.160  31.442  22.675  1.00 20.78           O
ATOM   2114  CB  MET A 275      32.367  28.695  23.589  1.00 23.06           C
ATOM   2115  CG  MET A 275      32.937  28.734  24.966  1.00 27.00           C
ATOM   2116  SD  MET A 275      34.545  27.926  24.991  1.00 33.74           S
ATOM   2117  CE  MET A 275      35.263  28.479  23.499  1.00 32.50           C
ATOM   2118  N   TYR A 276      30.583  31.211  24.832  1.00 21.96           N
ATOM   2119  CA  TYR A 276      30.485  32.656  25.138  1.00 23.15           C
ATOM   2120  C   TYR A 276      29.256  33.365  24.546  1.00 22.39           C
ATOM   2121  O   TYR A 276      28.989  34.496  24.899  1.00 22.58           O
ATOM   2122  CB  TYR A 276      31.776  33.409  24.760  1.00 23.80           C
ATOM   2123  CG  TYR A 276      32.904  33.136  25.729  1.00 28.82           C
ATOM   2124  CD1 TYR A 276      32.940  33.756  26.951  1.00 32.73           C
ATOM   2125  CD2 TYR A 276      33.935  32.246  25.415  1.00 35.83           C
ATOM   2126  CE1 TYR A 276      33.956  33.507  27.864  1.00 35.96           C
ATOM   2127  CE2 TYR A 276      34.975  31.992  26.336  1.00 38.59           C
ATOM   2128  CZ  TYR A 276      34.958  32.628  27.562  1.00 38.60           C
ATOM   2129  OH  TYR A 276      35.951  32.421  28.513  1.00 45.18           O
ATOM   2130  N   TRP A 277      28.488  32.709  23.684  1.00 21.71           N
ATOM   2131  CA  TRP A 277      27.281  33.350  23.149  1.00 21.24           C
ATOM   2132  C   TRP A 277      26.184  33.278  24.152  1.00 20.90           C
ATOM   2133  O   TRP A 277      25.914  32.217  24.708  1.00 21.96           O
ATOM   2134  CB  TRP A 277      26.790  32.711  21.856  1.00 21.01           C
ATOM   2135  CG  TRP A 277      27.547  33.166  20.670  1.00 19.98           C
ATOM   2136  CD1 TRP A 277      28.875  33.013  20.462  1.00 17.90           C
ATOM   2137  CD2 TRP A 277      27.030  33.832  19.519  1.00 19.76           C
ATOM   2138  NE1 TRP A 277      29.218  33.533  19.247  1.00 18.64           N
ATOM   2139  CE2 TRP A 277      28.106  34.071  18.662  1.00 18.29           C
ATOM   2140  CE3 TRP A 277      25.764  34.305  19.151  1.00 20.56           C
ATOM   2141  CZ2 TRP A 277      27.963  34.716  17.442  1.00 19.63           C
ATOM   2142  CZ3 TRP A 277      25.624  34.950  17.943  1.00 21.16           C
ATOM   2143  CH2 TRP A 277      26.720  35.137  17.095  1.00 19.92           C
ATOM   2144  N   TRP A 278      25.574  34.426  24.405  1.00 20.32           N
ATOM   2145  CA  TRP A 278      24.452  34.533  25.316  1.00 20.13           C
ATOM   2146  C   TRP A 278      23.268  33.787  24.741  1.00 19.99           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2147 | O | TRP | A | 278 | 23.083 | 33.758 | 23.538 | 1.00 | 20.42 | O |
| ATOM | 2148 | CB | TRP | A | 278 | 24.025 | 35.999 | 25.441 | 1.00 | 20.65 | C |
| ATOM | 2149 | CG | TRP | A | 278 | 25.031 | 36.864 | 26.107 | 1.00 | 20.56 | C |
| ATOM | 2150 | CD1 | TRP | A | 278 | 26.078 | 37.526 | 25.519 | 1.00 | 19.63 | C |
| ATOM | 2151 | CD2 | TRP | A | 278 | 25.096 | 37.160 | 27.501 | 1.00 | 19.59 | C |
| ATOM | 2152 | NE1 | TRP | A | 278 | 26.772 | 38.233 | 26.469 | 1.00 | 20.70 | N |
| ATOM | 2153 | CE2 | TRP | A | 278 | 26.191 | 38.012 | 27.699 | 1.00 | 20.10 | C |
| ATOM | 2154 | CE3 | TRP | A | 278 | 24.318 | 36.811 | 28.601 | 1.00 | 20.98 | C |
| ATOM | 2155 | CZ2 | TRP | A | 278 | 26.527 | 38.516 | 28.951 | 1.00 | 20.24 | C |
| ATOM | 2156 | CZ3 | TRP | A | 278 | 24.668 | 37.299 | 29.849 | 1.00 | 23.26 | C |
| ATOM | 2157 | CH2 | TRP | A | 278 | 25.759 | 38.146 | 30.011 | 1.00 | 20.41 | C |
| ATOM | 2158 | N | HIS | A | 279 | 22.463 | 33.194 | 25.591 | 1.00 | 19.84 | N |
| ATOM | 2159 | CA | HIS | A | 279 | 21.269 | 32.530 | 25.122 | 1.00 | 20.78 | C |
| ATOM | 2160 | C | HIS | A | 279 | 20.202 | 32.495 | 26.192 | 1.00 | 20.37 | C |
| ATOM | 2161 | O | HIS | A | 279 | 20.479 | 32.275 | 27.370 | 1.00 | 20.66 | O |
| ATOM | 2162 | CB | HIS | A | 279 | 21.540 | 31.098 | 24.604 | 1.00 | 20.86 | C |
| ATOM | 2163 | CG | HIS | A | 279 | 22.349 | 30.238 | 25.528 | 1.00 | 21.83 | C |
| ATOM | 2164 | ND1 | HIS | A | 279 | 23.720 | 30.324 | 25.608 | 1.00 | 23.19 | N |
| ATOM | 2165 | CD2 | HIS | A | 279 | 21.988 | 29.240 | 26.371 | 1.00 | 23.96 | C |
| ATOM | 2166 | CE1 | HIS | A | 279 | 24.175 | 29.411 | 26.449 | 1.00 | 22.20 | C |
| ATOM | 2167 | NE2 | HIS | A | 279 | 23.144 | 28.747 | 26.940 | 1.00 | 23.84 | N |
| ATOM | 2168 | N | HIS | A | 280 | 18.994 | 32.718 | 25.711 | 1.00 | 20.90 | N |
| ATOM | 2169 | CA | HIS | A | 280 | 17.742 | 32.758 | 26.441 | 1.00 | 21.22 | C |
| ATOM | 2170 | C | HIS | A | 280 | 16.910 | 31.676 | 25.793 | 1.00 | 21.42 | C |
| ATOM | 2171 | O | HIS | A | 280 | 16.749 | 31.685 | 24.580 | 1.00 | 21.70 | O |
| ATOM | 2172 | CB | HIS | A | 280 | 17.099 | 34.124 | 26.224 | 1.00 | 21.04 | C |
| ATOM | 2173 | CG | HIS | A | 280 | 15.632 | 34.168 | 26.489 | 1.00 | 21.54 | C |
| ATOM | 2174 | ND1 | HIS | A | 280 | 15.096 | 34.836 | 27.571 | 1.00 | 22.76 | N |
| ATOM | 2175 | CD2 | HIS | A | 280 | 14.581 | 33.660 | 25.802 | 1.00 | 22.74 | C |
| ATOM | 2176 | CE1 | HIS | A | 280 | 13.779 | 34.721 | 27.546 | 1.00 | 23.23 | C |
| ATOM | 2177 | NE2 | HIS | A | 280 | 13.441 | 34.014 | 26.482 | 1.00 | 23.05 | N |
| ATOM | 2178 | N | ILE | A | 281 | 16.367 | 30.755 | 26.584 | 1.00 | 22.31 | N |
| ATOM | 2179 | CA | ILE | A | 281 | 15.649 | 29.599 | 26.040 | 1.00 | 22.39 | C |
| ATOM | 2180 | C | ILE | A | 281 | 14.304 | 29.443 | 26.722 | 1.00 | 22.72 | C |
| ATOM | 2181 | O | ILE | A | 281 | 14.216 | 29.419 | 27.945 | 1.00 | 22.70 | O |
| ATOM | 2182 | CB | ILE | A | 281 | 16.527 | 28.336 | 26.189 | 1.00 | 22.98 | C |
| ATOM | 2183 | CG1 | ILE | A | 281 | 17.771 | 28.504 | 25.305 | 1.00 | 24.90 | C |
| ATOM | 2184 | CG2 | ILE | A | 281 | 15.770 | 27.059 | 25.771 | 1.00 | 21.60 | C |
| ATOM | 2185 | CD1 | ILE | A | 281 | 18.795 | 27.556 | 25.554 | 1.00 | 27.31 | C |
| ATOM | 2186 | N | GLU | A | 282 | 13.252 | 29.350 | 25.920 | 1.00 | 22.93 | N |
| ATOM | 2187 | CA | GLU | A | 282 | 11.903 | 29.205 | 26.458 | 1.00 | 23.35 | C |
| ATOM | 2188 | C | GLU | A | 282 | 11.101 | 28.105 | 25.769 | 1.00 | 22.59 | C |
| ATOM | 2189 | O | GLU | A | 282 | 11.092 | 27.982 | 24.549 | 1.00 | 21.77 | O |
| ATOM | 2190 | CB | GLU | A | 282 | 11.144 | 30.538 | 26.393 | 1.00 | 23.47 | C |
| ATOM | 2191 | CG | GLU | A | 282 | 10.830 | 31.055 | 25.009 | 1.00 | 25.70 | C |
| ATOM | 2192 | CD | GLU | A | 282 | 10.281 | 32.483 | 25.023 | 1.00 | 25.79 | C |
| ATOM | 2193 | OE1 | GLU | A | 282 | 10.898 | 33.356 | 25.665 | 1.00 | 27.49 | O |
| ATOM | 2194 | OE2 | GLU | A | 282 | 9.241 | 32.740 | 24.391 | 1.00 | 26.03 | O |
| ATOM | 2195 | N | SER | A | 283 | 10.456 | 27.293 | 26.588 | 1.00 | 22.44 | N |
| ATOM | 2196 | CA | SER | A | 283 | 9.570 | 26.246 | 26.103 | 1.00 | 23.00 | C |
| ATOM | 2197 | C | SER | A | 283 | 8.256 | 26.916 | 25.753 | 1.00 | 23.56 | C |
| ATOM | 2198 | O | SER | A | 283 | 7.685 | 27.615 | 26.584 | 1.00 | 24.14 | O |
| ATOM | 2199 | CB | SER | A | 283 | 9.346 | 25.204 | 27.188 | 1.00 | 22.59 | C |
| ATOM | 2200 | OG | SER | A | 283 | 10.496 | 24.400 | 27.345 | 1.00 | 22.67 | O |
| ATOM | 2201 | N | LEU | A | 284 | 7.763 | 26.694 | 24.541 | 1.00 | 24.07 | N |
| ATOM | 2202 | CA | LEU | A | 284 | 6.581 | 27.412 | 24.070 | 1.00 | 24.80 | C |
| ATOM | 2203 | C | LEU | A | 284 | 5.386 | 27.324 | 25.004 | 1.00 | 24.51 | C |
| ATOM | 2204 | O | LEU | A | 284 | 5.098 | 26.271 | 25.602 | 1.00 | 23.93 | O |
| ATOM | 2205 | CB | LEU | A | 284 | 6.161 | 26.947 | 22.682 | 1.00 | 25.09 | C |
| ATOM | 2206 | CG | LEU | A | 284 | 7.185 | 27.083 | 21.555 | 1.00 | 26.46 | C |
| ATOM | 2207 | CD1 | LEU | A | 284 | 6.475 | 27.236 | 20.215 | 1.00 | 28.29 | C |

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ATOM   2208  CD2 LEU A 284       8.123  28.188  21.775  1.00 26.10           C
ATOM   2209  N   LEU A 285       4.718  28.463  25.136  1.00 24.41           N
ATOM   2210  CA  LEU A 285       3.506  28.554  25.930  1.00 24.83           C
ATOM   2211  C   LEU A 285       2.526  27.583  25.323  1.00 24.68           C
ATOM   2212  O   LEU A 285       2.393  27.516  24.110  1.00 24.08           O
ATOM   2213  CB  LEU A 285       2.927  29.961  25.872  1.00 24.79           C
ATOM   2214  CG  LEU A 285       3.825  31.078  26.397  1.00 25.19           C
ATOM   2215  CD1 LEU A 285       3.298  32.434  25.954  1.00 26.02           C
ATOM   2216  CD2 LEU A 285       3.925  30.999  27.898  1.00 26.27           C
ATOM   2217  N   ASN A 286       1.867  26.815  26.173  1.00 25.20           N
ATOM   2218  CA  ASN A 286       0.867  25.848  25.730  1.00 25.85           C
ATOM   2219  C   ASN A 286       1.371  24.791  24.742  1.00 25.23           C
ATOM   2220  O   ASN A 286       0.594  24.267  23.965  1.00 24.38           O
ATOM   2221  CB  ASN A 286      -0.319  26.599  25.124  1.00 26.54           C
ATOM   2222  CG  ASN A 286      -0.957  27.546  26.109  1.00 29.40           C
ATOM   2223  OD1 ASN A 286      -1.478  27.118  27.140  1.00 33.49           O
ATOM   2224  ND2 ASN A 286      -0.893  28.843  25.821  1.00 33.58           N
ATOM   2225  N   GLY A 287       2.669  24.487  24.774  1.00 24.55           N
ATOM   2226  CA  GLY A 287       3.243  23.518  23.863  1.00 24.10           C
ATOM   2227  C   GLY A 287       3.524  22.167  24.487  1.00 23.80           C
ATOM   2228  O   GLY A 287       4.110  21.301  23.838  1.00 24.10           O
ATOM   2229  N   GLY A 288       3.100  21.971  25.734  1.00 23.32           N
ATOM   2230  CA  GLY A 288       3.360  20.730  26.439  1.00 23.24           C
ATOM   2231  C   GLY A 288       4.808  20.673  26.903  1.00 23.49           C
ATOM   2232  O   GLY A 288       5.548  21.646  26.741  1.00 22.86           O
ATOM   2233  N   ILE A 289       5.220  19.539  27.462  1.00 23.36           N
ATOM   2234  CA  ILE A 289       6.571  19.406  27.983  1.00 23.99           C
ATOM   2235  C   ILE A 289       7.601  19.374  26.874  1.00 23.28           C
ATOM   2236  O   ILE A 289       7.324  18.958  25.755  1.00 23.68           O
ATOM   2237  CB  ILE A 289       6.750  18.123  28.817  1.00 24.68           C
ATOM   2238  CG1 ILE A 289       6.819  16.912  27.901  1.00 26.90           C
ATOM   2239  CG2 ILE A 289       5.648  17.983  29.885  1.00 25.75           C
ATOM   2240  CD1 ILE A 289       7.294  15.640  28.613  1.00 29.37           C
ATOM   2241  N   THR A 290       8.811  19.790  27.210  1.00 22.42           N
ATOM   2242  CA  THR A 290       9.904  19.768  26.264  1.00 21.38           C
ATOM   2243  C   THR A 290      11.030  18.880  26.774  1.00 20.56           C
ATOM   2244  O   THR A 290      11.243  18.743  27.986  1.00 19.81           O
ATOM   2245  CB  THR A 290      10.461  21.175  26.053  1.00 21.70           C
ATOM   2246  OG1 THR A 290      10.823  21.761  27.308  1.00 20.15           O
ATOM   2247  CG2 THR A 290       9.405  22.108  25.460  1.00 21.76           C
ATOM   2248  N   ILE A 291      11.757  18.296  25.841  1.00 19.36           N
ATOM   2249  CA  ILE A 291      12.903  17.503  26.190  1.00 19.73           C
ATOM   2250  C   ILE A 291      14.044  17.865  25.286  1.00 19.29           C
ATOM   2251  O   ILE A 291      13.862  17.976  24.083  1.00 19.81           O
ATOM   2252  CB  ILE A 291      12.598  15.992  26.085  1.00 20.08           C
ATOM   2253  CG1 ILE A 291      11.467  15.609  27.044  1.00 20.06           C
ATOM   2254  CG2 ILE A 291      13.873  15.214  26.378  1.00 20.21           C
ATOM   2255  CD1 ILE A 291      11.028  14.131  26.931  1.00 21.77           C
ATOM   2256  N   THR A 292      15.215  18.070  25.882  1.00 18.95           N
ATOM   2257  CA  THR A 292      16.406  18.407  25.156  1.00 19.17           C
ATOM   2258  C   THR A 292      17.589  17.691  25.753  1.00 19.18           C
ATOM   2259  O   THR A 292      17.671  17.497  26.965  1.00 19.21           O
ATOM   2260  CB  THR A 292      16.703  19.937  25.259  1.00 19.83           C
ATOM   2261  OG1 THR A 292      15.559  20.724  24.879  1.00 20.23           O
ATOM   2262  CG2 THR A 292      17.787  20.350  24.270  1.00 20.15           C
ATOM   2263  N   VAL A 293      18.530  17.314  24.903  1.00 19.25           N
ATOM   2264  CA  VAL A 293      19.809  16.824  25.387  1.00 19.51           C
ATOM   2265  C   VAL A 293      20.912  17.667  24.749  1.00 19.58           C
ATOM   2266  O   VAL A 293      20.962  17.792  23.535  1.00 18.47           O
ATOM   2267  CB  VAL A 293      20.024  15.345  25.063  1.00 19.73           C
ATOM   2268  CG1 VAL A 293      21.490  14.951  25.250  1.00 20.24           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2269 | CG2 | VAL | A | 293 | 19.146 | 14.478 | 25.968 | 1.00 | 20.65 | C |
| ATOM | 2270 | N | ASN | A | 294 | 21.766 | 18.277 | 25.569 | 1.00 | 19.85 | N |
| ATOM | 2271 | CA | ASN | A | 294 | 22.882 | 19.057 | 25.039 | 1.00 | 20.26 | C |
| ATOM | 2272 | C | ASN | A | 294 | 24.179 | 18.232 | 25.052 | 1.00 | 20.35 | C |
| ATOM | 2273 | O | ASN | A | 294 | 24.233 | 17.131 | 25.634 | 1.00 | 21.82 | O |
| ATOM | 2274 | CB | ASN | A | 294 | 23.008 | 20.443 | 25.727 | 1.00 | 20.82 | C |
| ATOM | 2275 | CG | ASN | A | 294 | 23.676 | 20.388 | 27.102 | 1.00 | 21.84 | C |
| ATOM | 2276 | OD1 | ASN | A | 294 | 24.209 | 19.354 | 27.495 | 1.00 | 21.66 | O |
| ATOM | 2277 | ND2 | ASN | A | 294 | 23.630 | 21.519 | 27.849 | 1.00 | 21.23 | N |
| ATOM | 2278 | N | PHE | A | 295 | 25.186 | 18.729 | 24.346 | 1.00 | 20.69 | N |
| ATOM | 2279 | CA | PHE | A | 295 | 26.490 | 18.095 | 24.233 | 1.00 | 20.46 | C |
| ATOM | 2280 | C | PHE | A | 295 | 27.452 | 19.240 | 24.494 | 1.00 | 21.42 | C |
| ATOM | 2281 | O | PHE | A | 295 | 27.573 | 20.167 | 23.653 | 1.00 | 20.85 | O |
| ATOM | 2282 | CB | PHE | A | 295 | 26.728 | 17.569 | 22.814 | 1.00 | 20.62 | C |
| ATOM | 2283 | CG | PHE | A | 295 | 25.898 | 16.366 | 22.440 | 1.00 | 21.15 | C |
| ATOM | 2284 | CD1 | PHE | A | 295 | 24.526 | 16.468 | 22.247 | 1.00 | 21.98 | C |
| ATOM | 2285 | CD2 | PHE | A | 295 | 26.498 | 15.130 | 22.256 | 1.00 | 19.31 | C |
| ATOM | 2286 | CE1 | PHE | A | 295 | 23.791 | 15.343 | 21.902 | 1.00 | 19.77 | C |
| ATOM | 2287 | CE2 | PHE | A | 295 | 25.762 | 14.037 | 21.885 | 1.00 | 17.96 | C |
| ATOM | 2288 | CZ | PHE | A | 295 | 24.424 | 14.138 | 21.720 | 1.00 | 17.87 | C |
| ATOM | 2289 | N | TRP | A | 296 | 28.123 | 19.196 | 25.645 | 1.00 | 21.19 | N |
| ATOM | 2290 | CA | TRP | A | 296 | 29.023 | 20.275 | 26.050 | 1.00 | 21.46 | C |
| ATOM | 2291 | C | TRP | A | 296 | 30.481 | 19.834 | 25.873 | 1.00 | 21.42 | C |
| ATOM | 2292 | O | TRP | A | 296 | 30.898 | 18.795 | 26.387 | 1.00 | 21.96 | O |
| ATOM | 2293 | CB | TRP | A | 296 | 28.760 | 20.669 | 27.498 | 1.00 | 21.13 | C |
| ATOM | 2294 | CG | TRP | A | 296 | 27.853 | 21.859 | 27.710 | 1.00 | 21.95 | C |
| ATOM | 2295 | CD1 | TRP | A | 296 | 27.797 | 22.987 | 26.955 | 1.00 | 23.23 | C |
| ATOM | 2296 | CD2 | TRP | A | 296 | 26.935 | 22.067 | 28.797 | 1.00 | 22.27 | C |
| ATOM | 2297 | NE1 | TRP | A | 296 | 26.882 | 23.869 | 27.478 | 1.00 | 22.26 | N |
| ATOM | 2298 | CE2 | TRP | A | 296 | 26.336 | 23.329 | 28.607 | 1.00 | 22.53 | C |
| ATOM | 2299 | CE3 | TRP | A | 296 | 26.531 | 21.298 | 29.894 | 1.00 | 24.83 | C |
| ATOM | 2300 | CZ2 | TRP | A | 296 | 25.362 | 23.840 | 29.463 | 1.00 | 22.34 | C |
| ATOM | 2301 | CZ3 | TRP | A | 296 | 25.557 | 21.810 | 30.754 | 1.00 | 24.59 | C |
| ATOM | 2302 | CH2 | TRP | A | 296 | 24.993 | 23.075 | 30.531 | 1.00 | 23.75 | C |
| ATOM | 2303 | N | TYR | A | 297 | 31.235 | 20.632 | 25.126 | 1.00 | 21.64 | N |
| ATOM | 2304 | CA | TYR | A | 297 | 32.633 | 20.361 | 24.845 | 1.00 | 21.81 | C |
| ATOM | 2305 | C | TYR | A | 297 | 33.482 | 21.523 | 25.320 | 1.00 | 22.41 | C |
| ATOM | 2306 | O | TYR | A | 297 | 33.110 | 22.682 | 25.146 | 1.00 | 21.78 | O |
| ATOM | 2307 | CB | TYR | A | 297 | 32.862 | 20.198 | 23.344 | 1.00 | 21.49 | C |
| ATOM | 2308 | CG | TYR | A | 297 | 32.287 | 18.943 | 22.761 | 1.00 | 21.77 | C |
| ATOM | 2309 | CD1 | TYR | A | 297 | 30.934 | 18.870 | 22.415 | 1.00 | 21.68 | C |
| ATOM | 2310 | CD2 | TYR | A | 297 | 33.083 | 17.841 | 22.526 | 1.00 | 19.80 | C |
| ATOM | 2311 | CE1 | TYR | A | 297 | 30.405 | 17.734 | 21.890 | 1.00 | 22.16 | C |
| ATOM | 2312 | CE2 | TYR | A | 297 | 32.555 | 16.690 | 21.993 | 1.00 | 20.99 | C |
| ATOM | 2313 | CZ | TYR | A | 297 | 31.215 | 16.637 | 21.686 | 1.00 | 21.46 | C |
| ATOM | 2314 | OH | TYR | A | 297 | 30.673 | 15.494 | 21.159 | 1.00 | 22.11 | O |
| ATOM | 2315 | N | LYS | A | 298 | 34.632 | 21.220 | 25.899 | 1.00 | 23.17 | N |
| ATOM | 2316 | CA | LYS | A | 298 | 35.566 | 22.273 | 26.288 | 1.00 | 24.45 | C |
| ATOM | 2317 | C | LYS | A | 298 | 36.074 | 22.912 | 25.021 | 1.00 | 24.21 | C |
| ATOM | 2318 | O | LYS | A | 298 | 36.264 | 22.228 | 24.025 | 1.00 | 23.35 | O |
| ATOM | 2319 | CB | LYS | A | 298 | 36.748 | 21.699 | 27.085 | 1.00 | 24.85 | C |
| ATOM | 2320 | CG | LYS | A | 298 | 36.436 | 21.416 | 28.552 | 1.00 | 28.00 | C |
| ATOM | 2321 | CD | LYS | A | 298 | 37.657 | 20.865 | 29.298 | 1.00 | 31.59 | C |
| ATOM | 2322 | CE | LYS | A | 298 | 37.309 | 20.447 | 30.730 | 1.00 | 33.77 | C |
| ATOM | 2323 | NZ | LYS | A | 298 | 38.406 | 19.627 | 31.367 | 1.00 | 36.02 | N |
| ATOM | 2324 | N | GLY | A | 299 | 36.317 | 24.216 | 25.056 | 1.00 | 25.28 | N |
| ATOM | 2325 | CA | GLY | A | 299 | 36.818 | 24.909 | 23.886 | 1.00 | 26.38 | C |
| ATOM | 2326 | C | GLY | A | 299 | 38.254 | 24.542 | 23.547 | 1.00 | 27.78 | C |
| ATOM | 2327 | O | GLY | A | 299 | 38.935 | 23.895 | 24.315 | 1.00 | 27.16 | O |
| ATOM | 2328 | N | ALA | A | 300 | 38.690 | 24.949 | 22.366 | 1.00 | 30.42 | N |
| ATOM | 2329 | CA | ALA | A | 300 | 40.062 | 24.762 | 21.918 | 1.00 | 32.93 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2330 | C | ALA | A | 300 | 41.021 | 25.544 | 22.819 | 1.00 | 35.12 | C |
| ATOM | 2331 | O | ALA | A | 300 | 40.597 | 26.337 | 23.646 | 1.00 | 34.87 | O |
| ATOM | 2332 | CB | ALA | A | 300 | 40.199 | 25.249 | 20.472 | 1.00 | 32.98 | C |
| ATOM | 2333 | N | PRO | A | 301 | 42.318 | 25.355 | 22.615 | 1.00 | 38.54 | N |
| ATOM | 2334 | CA | PRO | A | 301 | 43.347 | 26.012 | 23.440 | 1.00 | 40.37 | C |
| ATOM | 2335 | C | PRO | A | 301 | 43.548 | 27.484 | 23.102 | 1.00 | 41.99 | C |
| ATOM | 2336 | O | PRO | A | 301 | 43.379 | 27.853 | 21.950 | 1.00 | 42.88 | O |
| ATOM | 2337 | CB | PRO | A | 301 | 44.615 | 25.246 | 23.061 | 1.00 | 40.42 | C |
| ATOM | 2338 | CG | PRO | A | 301 | 44.397 | 24.879 | 21.638 | 1.00 | 39.87 | C |
| ATOM | 2339 | CD | PRO | A | 301 | 42.919 | 24.544 | 21.535 | 1.00 | 38.98 | C |
| ATOM | 2340 | N | THR | A | 302 | 43.915 | 28.293 | 24.090 | 1.00 | 44.60 | N |
| ATOM | 2341 | CA | THR | A | 302 | 44.209 | 29.725 | 23.912 | 1.00 | 46.30 | C |
| ATOM | 2342 | C | THR | A | 302 | 45.593 | 29.790 | 23.315 | 1.00 | 47.41 | C |
| ATOM | 2343 | O | THR | A | 302 | 46.534 | 29.388 | 23.992 | 1.00 | 47.96 | O |
| ATOM | 2344 | CB | THR | A | 302 | 44.242 | 30.391 | 25.294 | 1.00 | 46.57 | C |
| ATOM | 2345 | OG1 | THR | A | 302 | 42.941 | 30.320 | 25.895 | 1.00 | 48.00 | O |
| ATOM | 2346 | CG2 | THR | A | 302 | 44.526 | 31.869 | 25.199 | 1.00 | 47.24 | C |
| ATOM | 2347 | N | PRO | A | 303 | 45.782 | 30.336 | 22.112 | 1.00 | 48.55 | N |
| ATOM | 2348 | CA | PRO | A | 303 | 47.090 | 30.170 | 21.473 | 1.00 | 48.80 | C |
| ATOM | 2349 | C | PRO | A | 303 | 48.210 | 30.717 | 22.341 | 1.00 | 48.76 | C |
| ATOM | 2350 | O | PRO | A | 303 | 47.874 | 31.450 | 23.269 | 1.00 | 49.07 | O |
| ATOM | 2351 | CB | PRO | A | 303 | 46.967 | 30.980 | 20.185 | 1.00 | 49.07 | C |
| ATOM | 2352 | CG | PRO | A | 303 | 45.504 | 31.101 | 19.952 | 1.00 | 48.93 | C |
| ATOM | 2353 | CD | PRO | A | 303 | 44.916 | 31.243 | 21.330 | 1.00 | 48.62 | C |
| ATOM | 2354 | N | GLU | A | 307 | 46.795 | 36.776 | 18.436 | 1.00 | 52.62 | N |
| ATOM | 2355 | CA | GLU | A | 307 | 46.885 | 37.814 | 17.415 | 1.00 | 52.76 | C |
| ATOM | 2356 | C | GLU | A | 307 | 45.865 | 38.906 | 17.636 | 1.00 | 52.00 | C |
| ATOM | 2357 | O | GLU | A | 307 | 44.757 | 38.658 | 18.096 | 1.00 | 52.48 | O |
| ATOM | 2358 | CB | GLU | A | 307 | 46.686 | 37.246 | 15.996 | 1.00 | 53.32 | C |
| ATOM | 2359 | CG | GLU | A | 307 | 46.893 | 38.307 | 14.908 | 1.00 | 54.63 | C |
| ATOM | 2360 | CD | GLU | A | 307 | 46.862 | 37.764 | 13.487 | 1.00 | 56.43 | C |
| ATOM | 2361 | OE1 | GLU | A | 307 | 46.527 | 36.574 | 13.290 | 1.00 | 57.49 | O |
| ATOM | 2362 | OE2 | GLU | A | 307 | 47.173 | 38.543 | 12.558 | 1.00 | 57.89 | O |
| ATOM | 2363 | N | TYR | A | 308 | 46.255 | 40.125 | 17.303 | 1.00 | 51.19 | N |
| ATOM | 2364 | CA | TYR | A | 308 | 45.367 | 41.267 | 17.405 | 1.00 | 50.55 | C |
| ATOM | 2365 | C | TYR | A | 308 | 44.747 | 41.494 | 16.039 | 1.00 | 49.51 | C |
| ATOM | 2366 | O | TYR | A | 308 | 45.300 | 41.053 | 15.028 | 1.00 | 49.70 | O |
| ATOM | 2367 | CB | TYR | A | 308 | 46.151 | 42.485 | 17.867 | 1.00 | 50.82 | C |
| ATOM | 2368 | CG | TYR | A | 308 | 46.702 | 42.286 | 19.259 | 1.00 | 52.47 | C |
| ATOM | 2369 | CD1 | TYR | A | 308 | 45.949 | 42.632 | 20.373 | 1.00 | 53.15 | C |
| ATOM | 2370 | CD2 | TYR | A | 308 | 47.948 | 41.696 | 19.462 | 1.00 | 53.79 | C |
| ATOM | 2371 | CE1 | TYR | A | 308 | 46.426 | 42.426 | 21.643 | 1.00 | 54.22 | C |
| ATOM | 2372 | CE2 | TYR | A | 308 | 48.437 | 41.487 | 20.736 | 1.00 | 54.76 | C |
| ATOM | 2373 | CZ | TYR | A | 308 | 47.670 | 41.857 | 21.824 | 1.00 | 55.10 | C |
| ATOM | 2374 | OH | TYR | A | 308 | 48.146 | 41.659 | 23.101 | 1.00 | 56.68 | O |
| ATOM | 2375 | N | PRO | A | 309 | 43.584 | 42.135 | 15.987 | 1.00 | 47.88 | N |
| ATOM | 2376 | CA | PRO | A | 309 | 42.843 | 42.621 | 17.169 | 1.00 | 46.21 | C |
| ATOM | 2377 | C | PRO | A | 309 | 42.139 | 41.503 | 17.952 | 1.00 | 43.75 | C |
| ATOM | 2378 | O | PRO | A | 309 | 41.768 | 40.503 | 17.369 | 1.00 | 44.10 | O |
| ATOM | 2379 | CB | PRO | A | 309 | 41.804 | 43.566 | 16.562 | 1.00 | 46.39 | C |
| ATOM | 2380 | CG | PRO | A | 309 | 41.610 | 43.069 | 15.128 | 1.00 | 47.65 | C |
| ATOM | 2381 | CD | PRO | A | 309 | 42.899 | 42.431 | 14.716 | 1.00 | 48.06 | C |
| ATOM | 2382 | N | LEU | A | 310 | 41.973 | 41.672 | 19.256 | 1.00 | 40.94 | N |
| ATOM | 2383 | CA | LEU | A | 310 | 41.349 | 40.650 | 20.093 | 1.00 | 38.75 | C |
| ATOM | 2384 | C | LEU | A | 310 | 39.863 | 40.491 | 19.817 | 1.00 | 36.87 | C |
| ATOM | 2385 | O | LEU | A | 310 | 39.148 | 41.474 | 19.610 | 1.00 | 37.02 | O |
| ATOM | 2386 | CB | LEU | A | 310 | 41.499 | 41.017 | 21.566 | 1.00 | 38.63 | C |
| ATOM | 2387 | CG | LEU | A | 310 | 42.571 | 40.351 | 22.435 | 1.00 | 37.97 | C |
| ATOM | 2388 | CD1 | LEU | A | 310 | 43.840 | 40.049 | 21.711 | 1.00 | 37.27 | C |
| ATOM | 2389 | CD2 | LEU | A | 310 | 42.836 | 41.234 | 23.637 | 1.00 | 37.27 | C |
| ATOM | 2390 | N | LYS | A | 311 | 39.392 | 39.254 | 19.847 | 1.00 | 34.04 | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2391 | CA | LYS | A | 311 | 37.972 | 38.998 | 19.702 | 1.00 | 32.20 | C |
| ATOM | 2392 | C | LYS | A | 311 | 37.208 | 39.376 | 20.968 | 1.00 | 30.33 | C |
| ATOM | 2393 | O | LYS | A | 311 | 37.760 | 39.421 | 22.072 | 1.00 | 29.17 | O |
| ATOM | 2394 | CB | LYS | A | 311 | 37.733 | 37.564 | 19.371 | 1.00 | 32.59 | C |
| ATOM | 2395 | N | ALA | A | 312 | 35.924 | 39.641 | 20.788 | 1.00 | 28.23 | N |
| ATOM | 2396 | CA | ALA | A | 312 | 35.074 | 40.011 | 21.895 | 1.00 | 27.38 | C |
| ATOM | 2397 | C | ALA | A | 312 | 35.148 | 38.973 | 23.005 | 1.00 | 26.28 | C |
| ATOM | 2398 | O | ALA | A | 312 | 35.271 | 39.334 | 24.172 | 1.00 | 24.54 | O |
| ATOM | 2399 | CB | ALA | A | 312 | 33.641 | 40.205 | 21.421 | 1.00 | 27.09 | C |
| ATOM | 2400 | N | HIS | A | 313 | 35.101 | 37.689 | 22.649 | 1.00 | 25.72 | N |
| ATOM | 2401 | CA | HIS | A | 313 | 35.086 | 36.669 | 23.674 | 1.00 | 25.82 | C |
| ATOM | 2402 | C | HIS | A | 313 | 36.399 | 36.609 | 24.428 | 1.00 | 24.79 | C |
| ATOM | 2403 | O | HIS | A | 313 | 36.428 | 36.183 | 25.557 | 1.00 | 24.19 | O |
| ATOM | 2404 | CB | HIS | A | 313 | 34.688 | 35.293 | 23.129 | 1.00 | 26.92 | C |
| ATOM | 2405 | CG | HIS | A | 313 | 35.741 | 34.641 | 22.303 | 1.00 | 29.84 | C |
| ATOM | 2406 | ND1 | HIS | A | 313 | 35.896 | 34.903 | 20.954 | 1.00 | 35.52 | N |
| ATOM | 2407 | CD2 | HIS | A | 313 | 36.702 | 33.746 | 22.627 | 1.00 | 33.54 | C |
| ATOM | 2408 | CE1 | HIS | A | 313 | 36.921 | 34.208 | 20.489 | 1.00 | 35.03 | C |
| ATOM | 2409 | NE2 | HIS | A | 313 | 37.424 | 33.491 | 21.481 | 1.00 | 35.78 | N |
| ATOM | 2410 | N | GLN | A | 314 | 37.479 | 37.042 | 23.803 | 1.00 | 24.43 | N |
| ATOM | 2411 | CA | GLN | A | 314 | 38.762 | 37.092 | 24.465 | 1.00 | 24.34 | C |
| ATOM | 2412 | C | GLN | A | 314 | 38.762 | 38.226 | 25.510 | 1.00 | 24.39 | C |
| ATOM | 2413 | O | GLN | A | 314 | 39.327 | 38.081 | 26.590 | 1.00 | 24.82 | O |
| ATOM | 2414 | CB | GLN | A | 314 | 39.882 | 37.290 | 23.439 | 1.00 | 24.47 | C |
| ATOM | 2415 | CG | GLN | A | 314 | 40.032 | 36.106 | 22.472 | 1.00 | 25.49 | C |
| ATOM | 2416 | CD | GLN | A | 314 | 41.036 | 36.362 | 21.366 | 1.00 | 25.52 | C |
| ATOM | 2417 | OE1 | GLN | A | 314 | 40.878 | 37.287 | 20.563 | 1.00 | 27.59 | O |
| ATOM | 2418 | NE2 | GLN | A | 314 | 42.078 | 35.553 | 21.330 | 1.00 | 28.22 | N |
| ATOM | 2419 | N | LYS | A | 315 | 38.113 | 39.337 | 25.196 | 1.00 | 23.51 | N |
| ATOM | 2420 | CA | LYS | A | 315 | 38.000 | 40.423 | 26.154 | 1.00 | 23.79 | C |
| ATOM | 2421 | C | LYS | A | 315 | 37.125 | 39.979 | 27.325 | 1.00 | 23.05 | C |
| ATOM | 2422 | O | LYS | A | 315 | 37.373 | 40.347 | 28.465 | 1.00 | 21.38 | O |
| ATOM | 2423 | CB | LYS | A | 315 | 37.421 | 41.667 | 25.504 | 1.00 | 24.09 | C |
| ATOM | 2424 | CG | LYS | A | 315 | 38.382 | 42.286 | 24.533 | 1.00 | 26.96 | C |
| ATOM | 2425 | CD | LYS | A | 315 | 37.849 | 43.552 | 23.947 | 1.00 | 31.28 | C |
| ATOM | 2426 | CE | LYS | A | 315 | 38.856 | 44.156 | 22.977 | 1.00 | 34.34 | C |
| ATOM | 2427 | NZ | LYS | A | 315 | 38.207 | 45.098 | 22.005 | 1.00 | 36.25 | N |
| ATOM | 2428 | N | VAL | A | 316 | 36.109 | 39.177 | 27.041 | 1.00 | 22.30 | N |
| ATOM | 2429 | CA | VAL | A | 316 | 35.276 | 38.673 | 28.113 | 1.00 | 22.39 | C |
| ATOM | 2430 | C | VAL | A | 316 | 36.124 | 37.800 | 29.063 | 1.00 | 22.29 | C |
| ATOM | 2431 | O | VAL | A | 316 | 36.040 | 37.932 | 30.274 | 1.00 | 21.27 | O |
| ATOM | 2432 | CB | VAL | A | 316 | 34.065 | 37.887 | 27.595 | 1.00 | 22.03 | C |
| ATOM | 2433 | CG1 | VAL | A | 316 | 33.309 | 37.282 | 28.750 | 1.00 | 21.64 | C |
| ATOM | 2434 | CG2 | VAL | A | 316 | 33.123 | 38.796 | 26.802 | 1.00 | 22.46 | C |
| ATOM | 2435 | N | ALA | A | 317 | 36.964 | 36.941 | 28.499 | 1.00 | 22.09 | N |
| ATOM | 2436 | CA | ALA | A | 317 | 37.848 | 36.086 | 29.295 | 1.00 | 21.98 | C |
| ATOM | 2437 | C | ALA | A | 317 | 38.783 | 36.916 | 30.164 | 1.00 | 21.61 | C |
| ATOM | 2438 | O | ALA | A | 317 | 39.042 | 36.573 | 31.300 | 1.00 | 21.05 | O |
| ATOM | 2439 | CB | ALA | A | 317 | 38.668 | 35.147 | 28.380 | 1.00 | 22.01 | C |
| ATOM | 2440 | N | ILE | A | 318 | 39.273 | 38.016 | 29.606 | 1.00 | 21.45 | N |
| ATOM | 2441 | CA | ILE | A | 318 | 40.162 | 38.917 | 30.318 | 1.00 | 21.24 | C |
| ATOM | 2442 | C | ILE | A | 318 | 39.431 | 39.511 | 31.524 | 1.00 | 21.38 | C |
| ATOM | 2443 | O | ILE | A | 318 | 39.937 | 39.462 | 32.646 | 1.00 | 20.76 | O |
| ATOM | 2444 | CB | ILE | A | 318 | 40.709 | 40.023 | 29.377 | 1.00 | 20.58 | C |
| ATOM | 2445 | CG1 | ILE | A | 318 | 41.715 | 39.434 | 28.400 | 1.00 | 21.19 | C |
| ATOM | 2446 | CG2 | ILE | A | 318 | 41.354 | 41.167 | 30.185 | 1.00 | 20.20 | C |
| ATOM | 2447 | CD1 | ILE | A | 318 | 42.223 | 40.419 | 27.353 | 1.00 | 21.35 | C |
| ATOM | 2448 | N | MET | A | 319 | 38.234 | 40.030 | 31.287 | 1.00 | 20.83 | N |
| ATOM | 2449 | CA | MET | A | 319 | 37.446 | 40.622 | 32.355 | 1.00 | 21.31 | C |
| ATOM | 2450 | C | MET | A | 319 | 37.154 | 39.617 | 33.454 | 1.00 | 21.52 | C |
| ATOM | 2451 | O | MET | A | 319 | 37.326 | 39.911 | 34.651 | 1.00 | 21.13 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2452 | CB | MET | A | 319 | 36.177 | 41.260 | 31.818 | 1.00 | 21.01 | C |
| ATOM | 2453 | CG | MET | A | 319 | 36.423 | 42.519 | 30.971 | 1.00 | 21.17 | C |
| ATOM | 2454 | SD | MET | A | 319 | 34.860 | 43.346 | 30.459 | 1.00 | 22.71 | S |
| ATOM | 2455 | CE | MET | A | 319 | 34.204 | 42.152 | 29.206 | 1.00 | 22.13 | C |
| ATOM | 2456 | N | ARG | A | 320 | 36.767 | 38.408 | 33.068 | 1.00 | 21.34 | N |
| ATOM | 2457 | CA | ARG | A | 320 | 36.532 | 37.399 | 34.075 | 1.00 | 21.12 | C |
| ATOM | 2458 | C | ARG | A | 320 | 37.801 | 37.186 | 34.898 | 1.00 | 21.25 | C |
| ATOM | 2459 | O | ARG | A | 320 | 37.747 | 37.064 | 36.122 | 1.00 | 21.48 | O |
| ATOM | 2460 | CB | ARG | A | 320 | 36.102 | 36.095 | 33.427 | 1.00 | 21.01 | C |
| ATOM | 2461 | CG | ARG | A | 320 | 34.723 | 36.145 | 32.741 | 1.00 | 20.63 | C |
| ATOM | 2462 | CD | ARG | A | 320 | 34.324 | 34.795 | 32.142 | 1.00 | 18.73 | C |
| ATOM | 2463 | NE | ARG | A | 320 | 34.225 | 33.824 | 33.225 | 1.00 | 19.25 | N |
| ATOM | 2464 | CZ | ARG | A | 320 | 33.247 | 33.809 | 34.115 | 1.00 | 19.86 | C |
| ATOM | 2465 | NH1 | ARG | A | 320 | 32.259 | 34.689 | 34.062 | 1.00 | 21.08 | N |
| ATOM | 2466 | NH2 | ARG | A | 320 | 33.263 | 32.923 | 35.081 | 1.00 | 23.29 | N |
| ATOM | 2467 | N | ASN | A | 321 | 38.947 | 37.123 | 34.231 | 1.00 | 20.94 | N |
| ATOM | 2468 | CA | ASN | A | 321 | 40.184 | 36.855 | 34.939 | 1.00 | 20.88 | C |
| ATOM | 2469 | C | ASN | A | 321 | 40.535 | 37.981 | 35.916 | 1.00 | 20.93 | C |
| ATOM | 2470 | O | ASN | A | 321 | 40.962 | 37.716 | 37.047 | 1.00 | 21.77 | O |
| ATOM | 2471 | CB | ASN | A | 321 | 41.324 | 36.552 | 33.958 | 1.00 | 21.04 | C |
| ATOM | 2472 | CG | ASN | A | 321 | 41.288 | 35.099 | 33.447 | 1.00 | 22.80 | C |
| ATOM | 2473 | OD1 | ASN | A | 321 | 40.924 | 34.193 | 34.185 | 1.00 | 23.97 | O |
| ATOM | 2474 | ND2 | ASN | A | 321 | 41.666 | 34.887 | 32.193 | 1.00 | 21.35 | N |
| ATOM | 2475 | N | ILE | A | 322 | 40.355 | 39.233 | 35.505 | 1.00 | 20.14 | N |
| ATOM | 2476 | CA | ILE | A | 322 | 40.633 | 40.336 | 36.408 | 1.00 | 20.06 | C |
| ATOM | 2477 | C | ILE | A | 322 | 39.742 | 40.196 | 37.650 | 1.00 | 19.42 | C |
| ATOM | 2478 | O | ILE | A | 322 | 40.207 | 40.345 | 38.767 | 1.00 | 18.73 | O |
| ATOM | 2479 | CB | ILE | A | 322 | 40.372 | 41.690 | 35.715 | 1.00 | 20.21 | C |
| ATOM | 2480 | CG1 | ILE | A | 322 | 41.320 | 41.894 | 34.535 | 1.00 | 21.54 | C |
| ATOM | 2481 | CG2 | ILE | A | 322 | 40.504 | 42.823 | 36.699 | 1.00 | 20.53 | C |
| ATOM | 2482 | CD1 | ILE | A | 322 | 42.806 | 41.798 | 34.868 | 1.00 | 24.56 | C |
| ATOM | 2483 | N | GLU | A | 323 | 38.458 | 39.904 | 37.454 | 1.00 | 18.94 | N |
| ATOM | 2484 | CA | GLU | A | 323 | 37.553 | 39.757 | 38.576 | 1.00 | 18.98 | C |
| ATOM | 2485 | C | GLU | A | 323 | 38.027 | 38.651 | 39.492 | 1.00 | 19.33 | C |
| ATOM | 2486 | O | GLU | A | 323 | 38.084 | 38.832 | 40.707 | 1.00 | 19.05 | O |
| ATOM | 2487 | CB | GLU | A | 323 | 36.113 | 39.538 | 38.106 | 1.00 | 19.25 | C |
| ATOM | 2488 | CG | GLU | A | 323 | 35.518 | 40.803 | 37.484 | 1.00 | 19.34 | C |
| ATOM | 2489 | CD | GLU | A | 323 | 34.143 | 40.616 | 36.855 | 1.00 | 18.71 | C |
| ATOM | 2490 | OE1 | GLU | A | 323 | 33.183 | 40.332 | 37.573 | 1.00 | 19.19 | O |
| ATOM | 2491 | OE2 | GLU | A | 323 | 34.024 | 40.805 | 35.636 | 1.00 | 19.56 | O |
| ATOM | 2492 | N | LYS | A | 324 | 38.425 | 37.528 | 38.908 | 1.00 | 19.55 | N |
| ATOM | 2493 | CA | LYS | A | 324 | 38.874 | 36.379 | 39.693 | 1.00 | 20.24 | C |
| ATOM | 2494 | C | LYS | A | 324 | 40.115 | 36.707 | 40.513 | 1.00 | 20.68 | C |
| ATOM | 2495 | O | LYS | A | 324 | 40.157 | 36.405 | 41.699 | 1.00 | 20.83 | O |
| ATOM | 2496 | CB | LYS | A | 324 | 39.175 | 35.175 | 38.789 | 1.00 | 20.07 | C |
| ATOM | 2497 | CG | LYS | A | 324 | 37.924 | 34.507 | 38.212 | 1.00 | 20.57 | C |
| ATOM | 2498 | CD | LYS | A | 324 | 38.331 | 33.318 | 37.350 | 1.00 | 20.28 | C |
| ATOM | 2499 | CE | LYS | A | 324 | 37.137 | 32.689 | 36.621 | 1.00 | 19.29 | C |
| ATOM | 2500 | NZ | LYS | A | 324 | 37.596 | 31.460 | 35.876 | 1.00 | 17.17 | N |
| ATOM | 2501 | N | MET | A | 325 | 41.112 | 37.320 | 39.885 | 1.00 | 21.21 | N |
| ATOM | 2502 | CA | MET | A | 325 | 42.366 | 37.657 | 40.568 | 1.00 | 22.87 | C |
| ATOM | 2503 | C | MET | A | 325 | 42.162 | 38.665 | 41.699 | 1.00 | 22.44 | C |
| ATOM | 2504 | O | MET | A | 325 | 42.763 | 38.560 | 42.771 | 1.00 | 22.08 | O |
| ATOM | 2505 | CB | MET | A | 325 | 43.380 | 38.232 | 39.572 | 1.00 | 23.32 | C |
| ATOM | 2506 | CG | MET | A | 325 | 43.993 | 37.195 | 38.671 | 1.00 | 27.47 | C |
| ATOM | 2507 | SD | MET | A | 325 | 44.795 | 37.924 | 37.197 | 1.00 | 35.56 | S |
| ATOM | 2508 | CE | MET | A | 325 | 45.664 | 39.189 | 38.009 | 1.00 | 34.71 | C |
| ATOM | 2509 | N | LEU | A | 326 | 41.309 | 39.641 | 41.452 | 1.00 | 22.71 | N |
| ATOM | 2510 | CA | LEU | A | 326 | 41.043 | 40.670 | 42.449 | 1.00 | 23.24 | C |
| ATOM | 2511 | C | LEU | A | 326 | 40.385 | 40.073 | 43.679 | 1.00 | 23.15 | C |
| ATOM | 2512 | O | LEU | A | 326 | 40.735 | 40.417 | 44.795 | 1.00 | 22.40 | O |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2513 | CB | LEU | A | 326 | 40.151 | 41.735 | 41.865 | 1.00 | 23.01 | C |
| ATOM | 2514 | CG | LEU | A | 326 | 40.677 | 43.139 | 41.625 | 1.00 | 25.86 | C |
| ATOM | 2515 | CD1 | LEU | A | 326 | 42.187 | 43.277 | 41.529 | 1.00 | 26.53 | C |
| ATOM | 2516 | CD2 | LEU | A | 326 | 39.986 | 43.672 | 40.377 | 1.00 | 25.54 | C |
| ATOM | 2517 | N | GLY | A | 327 | 39.441 | 39.164 | 43.460 | 1.00 | 23.29 | N |
| ATOM | 2518 | CA | GLY | A | 327 | 38.760 | 38.489 | 44.547 | 1.00 | 23.97 | C |
| ATOM | 2519 | C | GLY | A | 327 | 39.728 | 37.723 | 45.418 | 1.00 | 24.63 | C |
| ATOM | 2520 | O | GLY | A | 327 | 39.659 | 37.783 | 46.649 | 1.00 | 24.75 | O |
| ATOM | 2521 | N | GLU | A | 328 | 40.644 | 37.002 | 44.778 | 1.00 | 25.03 | N |
| ATOM | 2522 | CA | GLU | A | 328 | 41.671 | 36.265 | 45.506 | 1.00 | 26.08 | C |
| ATOM | 2523 | C | GLU | A | 328 | 42.661 | 37.180 | 46.223 | 1.00 | 25.43 | C |
| ATOM | 2524 | O | GLU | A | 328 | 43.029 | 36.926 | 47.367 | 1.00 | 25.16 | O |
| ATOM | 2525 | CB | GLU | A | 328 | 42.442 | 35.368 | 44.546 | 1.00 | 26.76 | C |
| ATOM | 2526 | CG | GLU | A | 328 | 41.576 | 34.278 | 43.947 | 1.00 | 30.36 | C |
| ATOM | 2527 | CD | GLU | A | 328 | 41.719 | 32.957 | 44.676 | 1.00 | 35.76 | C |
| ATOM | 2528 | OE1 | GLU | A | 328 | 42.091 | 32.986 | 45.878 | 1.00 | 38.79 | O |
| ATOM | 2529 | OE2 | GLU | A | 328 | 41.483 | 31.896 | 44.034 | 1.00 | 38.82 | O |
| ATOM | 2530 | N | ALA | A | 329 | 43.094 | 38.240 | 45.552 | 1.00 | 24.91 | N |
| ATOM | 2531 | CA | ALA | A | 329 | 44.102 | 39.119 | 46.134 | 1.00 | 24.95 | C |
| ATOM | 2532 | C | ALA | A | 329 | 43.535 | 39.929 | 47.285 | 1.00 | 24.94 | C |
| ATOM | 2533 | O | ALA | A | 329 | 44.197 | 40.147 | 48.276 | 1.00 | 24.57 | O |
| ATOM | 2534 | CB | ALA | A | 329 | 44.682 | 40.022 | 45.088 | 1.00 | 24.88 | C |
| ATOM | 2535 | N | LEU | A | 330 | 42.290 | 40.354 | 47.161 | 1.00 | 25.47 | N |
| ATOM | 2536 | CA | LEU | A | 330 | 41.672 | 41.133 | 48.219 | 1.00 | 26.16 | C |
| ATOM | 2537 | C | LEU | A | 330 | 41.212 | 40.265 | 49.379 | 1.00 | 26.80 | C |
| ATOM | 2538 | O | LEU | A | 330 | 40.994 | 40.761 | 50.471 | 1.00 | 27.00 | O |
| ATOM | 2539 | CB | LEU | A | 330 | 40.504 | 41.930 | 47.669 | 1.00 | 26.08 | C |
| ATOM | 2540 | CG | LEU | A | 330 | 40.954 | 42.981 | 46.653 | 1.00 | 26.04 | C |
| ATOM | 2541 | CD1 | LEU | A | 330 | 39.760 | 43.489 | 45.888 | 1.00 | 26.16 | C |
| ATOM | 2542 | CD2 | LEU | A | 330 | 41.688 | 44.134 | 47.353 | 1.00 | 26.65 | C |
| ATOM | 2543 | N | GLY | A | 331 | 41.037 | 38.977 | 49.126 | 1.00 | 27.87 | N |
| ATOM | 2544 | CA | GLY | A | 331 | 40.645 | 38.039 | 50.158 | 1.00 | 28.89 | C |
| ATOM | 2545 | C | GLY | A | 331 | 39.176 | 38.086 | 50.526 | 1.00 | 29.43 | C |
| ATOM | 2546 | O | GLY | A | 331 | 38.763 | 37.435 | 51.478 | 1.00 | 30.62 | O |
| ATOM | 2547 | N | ASN | A | 332 | 38.400 | 38.887 | 49.808 | 1.00 | 29.59 | N |
| ATOM | 2548 | CA | ASN | A | 332 | 36.963 | 38.995 | 50.023 | 1.00 | 29.64 | C |
| ATOM | 2549 | C | ASN | A | 332 | 36.367 | 39.500 | 48.718 | 1.00 | 29.00 | C |
| ATOM | 2550 | O | ASN | A | 332 | 36.649 | 40.605 | 48.303 | 1.00 | 28.70 | O |
| ATOM | 2551 | CB | ASN | A | 332 | 36.656 | 39.973 | 51.156 | 1.00 | 30.15 | C |
| ATOM | 2552 | CG | ASN | A | 332 | 35.162 | 40.094 | 51.441 | 1.00 | 31.82 | C |
| ATOM | 2553 | OD1 | ASN | A | 332 | 34.335 | 39.531 | 50.734 | 1.00 | 34.71 | O |
| ATOM | 2554 | ND2 | ASN | A | 332 | 34.818 | 40.818 | 52.504 | 1.00 | 35.11 | N |
| ATOM | 2555 | N | PRO | A | 333 | 35.528 | 38.706 | 48.081 | 1.00 | 28.53 | N |
| ATOM | 2556 | CA | PRO | A | 333 | 35.001 | 39.075 | 46.771 | 1.00 | 28.25 | C |
| ATOM | 2557 | C | PRO | A | 333 | 34.176 | 40.343 | 46.807 | 1.00 | 27.91 | C |
| ATOM | 2558 | O | PRO | A | 333 | 34.033 | 40.984 | 45.776 | 1.00 | 26.99 | O |
| ATOM | 2559 | CB | PRO | A | 333 | 34.120 | 37.893 | 46.368 | 1.00 | 28.16 | C |
| ATOM | 2560 | CG | PRO | A | 333 | 34.137 | 36.938 | 47.468 | 1.00 | 28.91 | C |
| ATOM | 2561 | CD | PRO | A | 333 | 35.022 | 37.415 | 48.561 | 1.00 | 28.96 | C |
| ATOM | 2562 | N | GLN | A | 334 | 33.638 | 40.701 | 47.965 | 1.00 | 27.80 | N |
| ATOM | 2563 | CA | GLN | A | 334 | 32.814 | 41.896 | 48.039 | 1.00 | 27.97 | C |
| ATOM | 2564 | C | GLN | A | 334 | 33.665 | 43.155 | 47.975 | 1.00 | 26.77 | C |
| ATOM | 2565 | O | GLN | A | 334 | 33.144 | 44.245 | 47.764 | 1.00 | 26.51 | O |
| ATOM | 2566 | CB | GLN | A | 334 | 31.906 | 41.867 | 49.278 | 1.00 | 28.98 | C |
| ATOM | 2567 | CG | GLN | A | 334 | 30.675 | 40.969 | 49.038 | 1.00 | 32.17 | C |
| ATOM | 2568 | CD | GLN | A | 334 | 29.661 | 40.962 | 50.175 | 1.00 | 35.54 | C |
| ATOM | 2569 | OE1 | GLN | A | 334 | 29.682 | 41.840 | 51.048 | 1.00 | 37.92 | O |
| ATOM | 2570 | NE2 | GLN | A | 334 | 28.760 | 39.961 | 50.163 | 1.00 | 36.72 | N |
| ATOM | 2571 | N | GLU | A | 335 | 34.974 | 43.007 | 48.132 | 1.00 | 25.19 | N |
| ATOM | 2572 | CA | GLU | A | 335 | 35.860 | 44.151 | 48.018 | 1.00 | 24.41 | C |
| ATOM | 2573 | C | GLU | A | 335 | 36.170 | 44.466 | 46.537 | 1.00 | 22.68 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2574 | O | GLU | A | 335 | 36.700 | 45.521 | 46.228 | 1.00 | 21.42 | O |
| ATOM | 2575 | CB | GLU | A | 335 | 37.150 | 43.928 | 48.835 | 1.00 | 24.98 | C |
| ATOM | 2576 | CG | GLU | A | 335 | 36.974 | 44.148 | 50.343 | 1.00 | 27.94 | C |
| ATOM | 2577 | CD | GLU | A | 335 | 38.264 | 44.055 | 51.139 | 1.00 | 31.85 | C |
| ATOM | 2578 | OE1 | GLU | A | 335 | 39.248 | 44.736 | 50.777 | 1.00 | 34.79 | O |
| ATOM | 2579 | OE2 | GLU | A | 335 | 38.298 | 43.312 | 52.158 | 1.00 | 36.87 | O |
| ATOM | 2580 | N | VAL | A | 336 | 35.809 | 43.566 | 45.625 | 1.00 | 21.32 | N |
| ATOM | 2581 | CA | VAL | A | 336 | 36.113 | 43.751 | 44.201 | 1.00 | 20.37 | C |
| ATOM | 2582 | C | VAL | A | 336 | 35.541 | 45.034 | 43.603 | 1.00 | 20.01 | C |
| ATOM | 2583 | O | VAL | A | 336 | 36.247 | 45.798 | 42.954 | 1.00 | 19.07 | O |
| ATOM | 2584 | CB | VAL | A | 336 | 35.647 | 42.554 | 43.371 | 1.00 | 20.60 | C |
| ATOM | 2585 | CG1 | VAL | A | 336 | 35.785 | 42.841 | 41.883 | 1.00 | 21.06 | C |
| ATOM | 2586 | CG2 | VAL | A | 336 | 36.463 | 41.316 | 43.743 | 1.00 | 20.68 | C |
| ATOM | 2587 | N | GLY | A | 337 | 34.260 | 45.275 | 43.842 | 1.00 | 19.61 | N |
| ATOM | 2588 | CA | GLY | A | 337 | 33.593 | 46.437 | 43.317 | 1.00 | 19.45 | C |
| ATOM | 2589 | C | GLY | A | 337 | 34.205 | 47.760 | 43.731 | 1.00 | 19.51 | C |
| ATOM | 2590 | O | GLY | A | 337 | 34.522 | 48.576 | 42.871 | 1.00 | 18.93 | O |
| ATOM | 2591 | N | PRO | A | 338 | 34.333 | 48.010 | 45.032 | 1.00 | 20.41 | N |
| ATOM | 2592 | CA | PRO | A | 338 | 34.959 | 49.253 | 45.503 | 1.00 | 20.40 | C |
| ATOM | 2593 | C | PRO | A | 338 | 36.368 | 49.500 | 44.923 | 1.00 | 20.13 | C |
| ATOM | 2594 | O | PRO | A | 338 | 36.674 | 50.630 | 44.548 | 1.00 | 19.20 | O |
| ATOM | 2595 | CB | PRO | A | 338 | 34.960 | 49.092 | 47.035 | 1.00 | 20.63 | C |
| ATOM | 2596 | CG | PRO | A | 338 | 33.749 | 48.261 | 47.298 | 1.00 | 21.17 | C |
| ATOM | 2597 | CD | PRO | A | 338 | 33.782 | 47.221 | 46.151 | 1.00 | 20.95 | C |
| ATOM | 2598 | N | LEU | A | 339 | 37.199 | 48.470 | 44.831 | 1.00 | 20.34 | N |
| ATOM | 2599 | CA | LEU | A | 339 | 38.518 | 48.655 | 44.234 | 1.00 | 20.55 | C |
| ATOM | 2600 | C | LEU | A | 339 | 38.382 | 49.060 | 42.768 | 1.00 | 20.06 | C |
| ATOM | 2601 | O | LEU | A | 339 | 39.020 | 50.019 | 42.330 | 1.00 | 19.61 | O |
| ATOM | 2602 | CB | LEU | A | 339 | 39.383 | 47.408 | 44.358 | 1.00 | 20.81 | C |
| ATOM | 2603 | CG | LEU | A | 339 | 40.855 | 47.618 | 43.943 | 1.00 | 22.54 | C |
| ATOM | 2604 | CD1 | LEU | A | 339 | 41.809 | 46.817 | 44.786 | 1.00 | 25.30 | C |
| ATOM | 2605 | CD2 | LEU | A | 339 | 41.035 | 47.209 | 42.496 | 1.00 | 23.17 | C |
| ATOM | 2606 | N | LEU | A | 340 | 37.526 | 48.361 | 42.023 | 1.00 | 19.51 | N |
| ATOM | 2607 | CA | LEU | A | 340 | 37.327 | 48.687 | 40.600 | 1.00 | 19.36 | C |
| ATOM | 2608 | C | LEU | A | 340 | 36.827 | 50.120 | 40.427 | 1.00 | 19.30 | C |
| ATOM | 2609 | O | LEU | A | 340 | 37.318 | 50.861 | 39.566 | 1.00 | 17.55 | O |
| ATOM | 2610 | CB | LEU | A | 340 | 36.361 | 47.721 | 39.952 | 1.00 | 19.31 | C |
| ATOM | 2611 | CG | LEU | A | 340 | 36.929 | 46.333 | 39.637 | 1.00 | 21.99 | C |
| ATOM | 2612 | CD1 | LEU | A | 340 | 35.842 | 45.506 | 39.069 | 1.00 | 22.03 | C |
| ATOM | 2613 | CD2 | LEU | A | 340 | 38.140 | 46.390 | 38.673 | 1.00 | 21.20 | C |
| ATOM | 2614 | N | ASN | A | 341 | 35.879 | 50.521 | 41.270 | 1.00 | 19.17 | N |
| ATOM | 2615 | CA | ASN | A | 341 | 35.369 | 51.887 | 41.232 | 1.00 | 20.20 | C |
| ATOM | 2616 | C | ASN | A | 341 | 36.465 | 52.914 | 41.530 | 1.00 | 19.98 | C |
| ATOM | 2617 | O | ASN | A | 341 | 36.598 | 53.920 | 40.848 | 1.00 | 19.61 | O |
| ATOM | 2618 | CB | ASN | A | 341 | 34.181 | 52.043 | 42.196 | 1.00 | 20.66 | C |
| ATOM | 2619 | CG | ASN | A | 341 | 32.898 | 51.459 | 41.619 | 1.00 | 24.17 | C |
| ATOM | 2620 | OD1 | ASN | A | 341 | 32.484 | 51.843 | 40.531 | 1.00 | 30.93 | O |
| ATOM | 2621 | ND2 | ASN | A | 341 | 32.294 | 50.499 | 42.317 | 1.00 | 26.37 | N |
| ATOM | 2622 | N | THR | A | 342 | 37.245 | 52.633 | 42.558 | 1.00 | 20.07 | N |
| ATOM | 2623 | CA | THR | A | 342 | 38.351 | 53.489 | 42.939 | 1.00 | 20.49 | C |
| ATOM | 2624 | C | THR | A | 342 | 39.322 | 53.613 | 41.763 | 1.00 | 20.27 | C |
| ATOM | 2625 | O | THR | A | 342 | 39.835 | 54.688 | 41.502 | 1.00 | 19.66 | O |
| ATOM | 2626 | CB | THR | A | 342 | 39.001 | 52.909 | 44.189 | 1.00 | 20.82 | C |
| ATOM | 2627 | OG1 | THR | A | 342 | 38.123 | 53.124 | 45.320 | 1.00 | 22.13 | O |
| ATOM | 2628 | CG2 | THR | A | 342 | 40.308 | 53.625 | 44.545 | 1.00 | 21.01 | C |
| ATOM | 2629 | N | MET | A | 343 | 39.517 | 52.525 | 41.024 | 1.00 | 20.30 | N |
| ATOM | 2630 | CA | MET | A | 343 | 40.402 | 52.543 | 39.873 | 1.00 | 20.66 | C |
| ATOM | 2631 | C | MET | A | 343 | 39.932 | 53.445 | 38.758 | 1.00 | 20.29 | C |
| ATOM | 2632 | O | MET | A | 343 | 40.750 | 54.119 | 38.129 | 1.00 | 19.31 | O |
| ATOM | 2633 | CB | MET | A | 343 | 40.560 | 51.157 | 39.270 | 1.00 | 20.76 | C |
| ATOM | 2634 | CG | MET | A | 343 | 41.810 | 50.453 | 39.625 | 1.00 | 23.39 | C |

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ATOM   2635  SD  MET A 343      42.247  49.059  38.524  1.00 25.69           S
ATOM   2636  CE  MET A 343      41.161  48.058  38.968  1.00 26.74           C
ATOM   2637  N   ILE A 344      38.631  53.438  38.466  1.00 20.76           N
ATOM   2638  CA  ILE A 344      38.167  54.187  37.312  1.00 21.23           C
ATOM   2639  C   ILE A 344      37.648  55.577  37.565  1.00 20.71           C
ATOM   2640  O   ILE A 344      37.763  56.403  36.666  1.00 20.65           O
ATOM   2641  CB  ILE A 344      37.109  53.400  36.458  1.00 22.07           C
ATOM   2642  CG1 ILE A 344      35.710  53.613  36.992  1.00 23.91           C
ATOM   2643  CG2 ILE A 344      37.482  51.943  36.352  1.00 24.35           C
ATOM   2644  CD1 ILE A 344      34.650  53.199  36.033  1.00 28.26           C
ATOM   2645  N   LYS A 345      37.069  55.886  38.726  1.00 20.84           N
ATOM   2646  CA  LYS A 345      36.482  57.231  38.817  1.00 21.15           C
ATOM   2647  C   LYS A 345      37.464  58.376  38.784  1.00 19.86           C
ATOM   2648  O   LYS A 345      38.459  58.429  39.517  1.00 19.23           O
ATOM   2649  CB  LYS A 345      35.438  57.451  39.922  1.00 22.66           C
ATOM   2650  CG  LYS A 345      35.562  56.714  41.190  1.00 27.82           C
ATOM   2651  CD  LYS A 345      34.214  56.021  41.489  1.00 30.51           C
ATOM   2652  CE  LYS A 345      33.398  56.782  42.502  1.00 32.51           C
ATOM   2653  NZ  LYS A 345      34.069  56.806  43.829  1.00 37.63           N
ATOM   2654  N   GLY A 346      37.143  59.307  37.899  1.00 18.18           N
ATOM   2655  CA  GLY A 346      37.978  60.453  37.644  1.00 17.22           C
ATOM   2656  C   GLY A 346      39.303  60.105  36.978  1.00 16.31           C
ATOM   2657  O   GLY A 346      40.172  60.949  36.889  1.00 16.63           O
ATOM   2658  N   ARG A 347      39.453  58.872  36.531  1.00 16.85           N
ATOM   2659  CA  ARG A 347      40.697  58.413  35.904  1.00 17.52           C
ATOM   2660  C   ARG A 347      40.469  57.811  34.502  1.00 17.57           C
ATOM   2661  O   ARG A 347      41.178  58.143  33.559  1.00 17.10           O
ATOM   2662  CB  ARG A 347      41.379  57.384  36.812  1.00 17.20           C
ATOM   2663  CG  ARG A 347      41.822  57.949  38.181  1.00 16.77           C
ATOM   2664  CD  ARG A 347      43.287  57.491  38.583  1.00 18.88           C
ATOM   2665  NE  ARG A 347      43.254  56.087  38.618  1.00 17.77           N
ATOM   2666  CZ  ARG A 347      44.115  55.220  38.149  1.00 16.11           C
ATOM   2667  NH1 ARG A 347      45.323  55.512  37.658  1.00 16.59           N
ATOM   2668  NH2 ARG A 347      43.734  53.978  38.276  1.00 13.22           N
ATOM   2669  N   TYR A 348      39.472  56.954  34.375  1.00 18.74           N
ATOM   2670  CA  TYR A 348      39.138  56.317  33.091  1.00 20.48           C
ATOM   2671  C   TYR A 348      37.674  56.499  32.671  1.00 21.75           C
ATOM   2672  O   TYR A 348      37.296  56.047  31.596  1.00 22.39           O
ATOM   2673  CB  TYR A 348      39.411  54.800  33.124  1.00 19.97           C
ATOM   2674  CG  TYR A 348      40.874  54.384  33.199  1.00 19.65           C
ATOM   2675  CD1 TYR A 348      41.661  54.310  32.054  1.00 18.48           C
ATOM   2676  CD2 TYR A 348      41.458  54.051  34.414  1.00 17.73           C
ATOM   2677  CE1 TYR A 348      42.986  53.921  32.122  1.00 19.00           C
ATOM   2678  CE2 TYR A 348      42.775  53.667  34.494  1.00 18.72           C
ATOM   2679  CZ  TYR A 348      43.543  53.600  33.339  1.00 18.96           C
ATOM   2680  OH  TYR A 348      44.856  53.203  33.419  1.00 17.77           O
ATOM   2681  N   ASN A 349      36.837  57.123  33.488  1.00 23.99           N
ATOM   2682  CA  ASN A 349      35.429  57.244  33.089  1.00 26.57           C
ATOM   2683  C   ASN A 349      34.947  58.611  32.689  1.00 27.62           C
ATOM   2684  O   ASN A 349      35.646  59.606  32.655  1.00 28.49           O
ATOM   2685  CB  ASN A 349      34.496  56.720  34.150  1.00 26.11           C
ATOM   2686  CG  ASN A 349      34.511  57.552  35.386  1.00 28.01           C
ATOM   2687  OD1 ASN A 349      35.282  58.518  35.517  1.00 29.49           O
ATOM   2688  ND2 ASN A 349      33.658  57.173  36.342  1.00 31.84           N
ATOM   2689  OXT ASN A 349      33.761  58.686  32.399  1.00 31.04           O
TER    2690      ASN A 349
ATOM   2691  N   LEU S 795      45.837  35.555  30.600  1.00 35.49           N
ATOM   2692  CA  LEU S 795      44.757  36.539  30.946  1.00 35.77           C
ATOM   2693  C   LEU S 795      43.580  36.250  30.030  1.00 35.54           C
ATOM   2694  O   LEU S 795      42.418  36.338  30.412  1.00 34.79           O
ATOM   2695  CB  LEU S 795      45.257  37.967  30.787  1.00 36.01           C
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| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2696 | CG | LEU | S | 795 | 44.695 | 38.978 | 31.791 | 1.00 | 37.16 | C |
| ATOM | 2697 | CD1 | LEU | S | 795 | 44.761 | 38.459 | 33.204 | 1.00 | 37.65 | C |
| ATOM | 2698 | CD2 | LEU | S | 795 | 45.450 | 40.289 | 31.718 | 1.00 | 38.07 | C |
| ATOM | 2699 | N | THR | S | 796 | 43.936 | 35.940 | 28.796 | 1.00 | 35.47 | N |
| ATOM | 2700 | CA | THR | S | 796 | 43.060 | 35.351 | 27.800 | 1.00 | 36.25 | C |
| ATOM | 2701 | C | THR | S | 796 | 42.644 | 33.888 | 28.079 | 1.00 | 35.84 | C |
| ATOM | 2702 | O | THR | S | 796 | 41.819 | 33.331 | 27.365 | 1.00 | 36.38 | O |
| ATOM | 2703 | CB | THR | S | 796 | 43.817 | 35.429 | 26.457 | 1.00 | 36.63 | C |
| ATOM | 2704 | OG1 | THR | S | 796 | 43.251 | 34.528 | 25.524 | 1.00 | 38.48 | O |
| ATOM | 2705 | CG2 | THR | S | 796 | 45.257 | 34.907 | 26.593 | 1.00 | 37.07 | C |
| ATOM | 2706 | N | SER | S | 797 | 43.197 | 33.251 | 29.101 | 1.00 | 35.44 | N |
| ATOM | 2707 | CA | SER | S | 797 | 42.835 | 31.860 | 29.377 | 1.00 | 35.29 | C |
| ATOM | 2708 | C | SER | S | 797 | 41.426 | 31.760 | 29.984 | 1.00 | 35.18 | C |
| ATOM | 2709 | O | SER | S | 797 | 40.925 | 32.701 | 30.611 | 1.00 | 33.96 | O |
| ATOM | 2710 | CB | SER | S | 797 | 43.856 | 31.189 | 30.291 | 1.00 | 35.17 | C |
| ATOM | 2711 | OG | SER | S | 797 | 43.716 | 31.654 | 31.624 | 1.00 | 36.65 | O |
| ATOM | 2712 | N | TYR | S | 798 | 40.789 | 30.611 | 29.790 | 1.00 | 35.36 | N |
| ATOM | 2713 | CA | TYR | S | 798 | 39.427 | 30.430 | 30.256 | 1.00 | 35.94 | C |
| ATOM | 2714 | C | TYR | S | 798 | 39.148 | 29.075 | 30.890 | 1.00 | 35.14 | C |
| ATOM | 2715 | O | TYR | S | 798 | 39.845 | 28.095 | 30.657 | 1.00 | 35.54 | O |
| ATOM | 2716 | CB | TYR | S | 798 | 38.440 | 30.707 | 29.120 | 1.00 | 36.37 | C |
| ATOM | 2717 | CG | TYR | S | 798 | 38.554 | 29.794 | 27.920 | 1.00 | 39.89 | C |
| ATOM | 2718 | CD1 | TYR | S | 798 | 39.587 | 29.934 | 26.996 | 1.00 | 42.41 | C |
| ATOM | 2719 | CD2 | TYR | S | 798 | 37.606 | 28.808 | 27.697 | 1.00 | 43.13 | C |
| ATOM | 2720 | CE1 | TYR | S | 798 | 39.681 | 29.095 | 25.893 | 1.00 | 43.97 | C |
| ATOM | 2721 | CE2 | TYR | S | 798 | 37.687 | 27.963 | 26.597 | 1.00 | 44.94 | C |
| ATOM | 2722 | CZ | TYR | S | 798 | 38.723 | 28.109 | 25.698 | 1.00 | 44.95 | C |
| ATOM | 2723 | OH | TYR | S | 798 | 38.781 | 27.270 | 24.613 | 1.00 | 44.37 | O |
| ATOM | 2724 | N | ASP | S | 799 | 38.108 | 29.046 | 31.709 | 1.00 | 34.54 | N |
| ATOM | 2725 | CA | ASP | S | 799 | 37.685 | 27.840 | 32.392 | 1.00 | 33.87 | C |
| ATOM | 2726 | C | ASP | S | 799 | 36.600 | 27.187 | 31.545 | 1.00 | 32.58 | C |
| ATOM | 2727 | O | ASP | S | 799 | 36.465 | 27.501 | 30.366 | 1.00 | 32.32 | O |
| ATOM | 2728 | CB | ASP | S | 799 | 37.140 | 28.208 | 33.770 | 1.00 | 34.50 | C |
| ATOM | 2729 | CG | ASP | S | 799 | 37.299 | 27.104 | 34.773 | 1.00 | 36.07 | C |
| ATOM | 2730 | OD1 | ASP | S | 799 | 36.790 | 25.986 | 34.551 | 1.00 | 37.15 | O |
| ATOM | 2731 | OD2 | ASP | S | 799 | 37.918 | 27.279 | 35.833 | 1.00 | 41.54 | O |
| ATOM | 2732 | N | CYS | S | 800 | 35.812 | 26.301 | 32.141 | 1.00 | 30.83 | N |
| ATOM | 2733 | CA | CYS | S | 800 | 34.798 | 25.586 | 31.392 | 1.00 | 29.83 | C |
| ATOM | 2734 | C | CYS | S | 800 | 33.490 | 25.511 | 32.161 | 1.00 | 29.15 | C |
| ATOM | 2735 | O | CYS | S | 800 | 32.794 | 24.502 | 32.092 | 1.00 | 28.68 | O |
| ATOM | 2736 | CB | CYS | S | 800 | 35.273 | 24.167 | 31.092 | 1.00 | 29.46 | C |
| ATOM | 2737 | SG | CYS | S | 800 | 35.576 | 23.194 | 32.601 | 1.00 | 30.36 | S |
| ATOM | 2738 | N | GLU | S | 801 | 33.152 | 26.578 | 32.874 | 1.00 | 28.36 | N |
| ATOM | 2739 | CA | GLU | S | 801 | 31.936 | 26.605 | 33.670 | 1.00 | 28.63 | C |
| ATOM | 2740 | C | GLU | S | 801 | 30.667 | 26.793 | 32.829 | 1.00 | 28.34 | C |
| ATOM | 2741 | O | GLU | S | 801 | 30.626 | 27.562 | 31.867 | 1.00 | 27.30 | O |
| ATOM | 2742 | CB | GLU | S | 801 | 32.038 | 27.688 | 34.751 | 1.00 | 28.61 | C |
| ATOM | 2743 | CG | GLU | S | 801 | 33.252 | 27.501 | 35.655 | 1.00 | 30.83 | C |
| ATOM | 2744 | CD | GLU | S | 801 | 33.188 | 28.346 | 36.907 | 1.00 | 32.58 | C |
| ATOM | 2745 | OE1 | GLU | S | 801 | 32.414 | 27.985 | 37.805 | 1.00 | 33.57 | O |
| ATOM | 2746 | OE2 | GLU | S | 801 | 33.910 | 29.362 | 36.989 | 1.00 | 33.97 | O |
| ATOM | 2747 | N | VAL | S | 802 | 29.627 | 26.062 | 33.212 | 1.00 | 28.85 | N |
| ATOM | 2748 | CA | VAL | S | 802 | 28.350 | 26.079 | 32.515 | 1.00 | 29.03 | C |
| ATOM | 2749 | C | VAL | S | 802 | 27.233 | 26.056 | 33.546 | 1.00 | 29.80 | C |
| ATOM | 2750 | O | VAL | S | 802 | 27.505 | 25.948 | 34.726 | 1.00 | 29.92 | O |
| ATOM | 2751 | CB | VAL | S | 802 | 28.221 | 24.834 | 31.606 | 1.00 | 28.44 | C |
| ATOM | 2752 | CG1 | VAL | S | 802 | 29.288 | 24.856 | 30.523 | 1.00 | 26.99 | C |
| ATOM | 2753 | CG2 | VAL | S | 802 | 28.333 | 23.551 | 32.428 | 1.00 | 29.08 | C |
| ATOM | 2754 | N | ASN | S | 803 | 25.978 | 26.135 | 33.111 | 1.00 | 31.09 | N |
| ATOM | 2755 | CA | ASN | S | 803 | 24.853 | 26.053 | 34.042 | 1.00 | 32.53 | C |
| ATOM | 2756 | C | ASN | S | 803 | 24.550 | 24.641 | 34.497 | 1.00 | 33.81 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2757 | O | ASN | S | 803 | 23.456 | 24.143 | 34.270 | 1.00 | 34.27 | O |
| ATOM | 2758 | CB | ASN | S | 803 | 23.575 | 26.659 | 33.463 | 1.00 | 32.29 | C |
| ATOM | 2759 | CG | ASN | S | 803 | 23.640 | 28.146 | 33.367 | 1.00 | 31.77 | C |
| ATOM | 2760 | OD1 | ASN | S | 803 | 24.688 | 28.741 | 33.616 | 1.00 | 33.47 | O |
| ATOM | 2761 | ND2 | ASN | S | 803 | 22.525 | 28.772 | 33.005 | 1.00 | 29.83 | N |
| ATOM | 2762 | N | ALA | S | 804 | 25.521 | 24.015 | 35.147 | 1.00 | 35.23 | N |
| ATOM | 2763 | CA | ALA | S | 804 | 25.365 | 22.689 | 35.740 | 1.00 | 36.86 | C |
| ATOM | 2764 | C | ALA | S | 804 | 26.577 | 22.452 | 36.638 | 1.00 | 37.98 | C |
| ATOM | 2765 | O | ALA | S | 804 | 27.660 | 22.949 | 36.360 | 1.00 | 37.44 | O |
| ATOM | 2766 | CB | ALA | S | 804 | 25.285 | 21.610 | 34.676 | 1.00 | 36.63 | C |
| ATOM | 2767 | N | PRO | S | 805 | 26.394 | 21.694 | 37.711 | 1.00 | 40.20 | N |
| ATOM | 2768 | CA | PRO | S | 805 | 27.495 | 21.381 | 38.635 | 1.00 | 41.46 | C |
| ATOM | 2769 | C | PRO | S | 805 | 28.572 | 20.511 | 37.983 | 1.00 | 42.51 | C |
| ATOM | 2770 | O | PRO | S | 805 | 28.342 | 19.931 | 36.938 | 1.00 | 43.07 | O |
| ATOM | 2771 | CB | PRO | S | 805 | 26.799 | 20.615 | 39.774 | 1.00 | 41.54 | C |
| ATOM | 2772 | CG | PRO | S | 805 | 25.506 | 20.116 | 39.185 | 1.00 | 41.29 | C |
| ATOM | 2773 | CD | PRO | S | 805 | 25.117 | 21.076 | 38.115 | 1.00 | 40.40 | C |
| ATOM | 2774 | N | ILE | S | 806 | 29.728 | 20.406 | 38.622 | 1.00 | 44.25 | N |
| ATOM | 2775 | CA | ILE | S | 806 | 30.854 | 19.627 | 38.099 | 1.00 | 44.96 | C |
| ATOM | 2776 | C | ILE | S | 806 | 30.770 | 18.169 | 38.532 | 1.00 | 45.18 | C |
| ATOM | 2777 | O | ILE | S | 806 | 29.902 | 17.801 | 39.323 | 1.00 | 45.78 | O |
| ATOM | 2778 | CB | ILE | S | 806 | 32.197 | 20.246 | 38.569 | 1.00 | 45.19 | C |
| ATOM | 2779 | CG1 | ILE | S | 806 | 32.412 | 20.018 | 40.070 | 1.00 | 46.10 | C |
| ATOM | 2780 | CG2 | ILE | S | 806 | 32.230 | 21.743 | 38.246 | 1.00 | 46.08 | C |
| ATOM | 2781 | CD1 | ILE | S | 806 | 33.740 | 20.574 | 40.597 | 1.00 | 46.98 | C |
| ATOM | 2782 | N | LEU | S | 812 | 29.934 | 8.629 | 39.561 | 1.00 | 43.80 | N |
| ATOM | 2783 | CA | LEU | S | 812 | 29.027 | 8.736 | 38.425 | 1.00 | 43.90 | C |
| ATOM | 2784 | C | LEU | S | 812 | 29,761 | 9.243 | 37.182 | 1.00 | 43.45 | C |
| ATOM | 2785 | O | LEU | S | 812 | 30.160 | 10.410 | 37.114 | 1.00 | 43.36 | O |
| ATOM | 2786 | CB | LEU | S | 812 | 27.862 | 9.678 | 38.757 | 1.00 | 44.22 | C |
| ATOM | 2787 | CG | LEU | S | 812 | 26.979 | 9.292 | 39.951 | 1.00 | 45.50 | C |
| ATOM | 2788 | CD1 | LEU | S | 812 | 25.871 | 10.341 | 40.144 | 1.00 | 46.20 | C |
| ATOM | 2789 | CD2 | LEU | S | 812 | 26.385 | 7.894 | 39.793 | 1.00 | 45.08 | C |
| ATOM | 2790 | N | LEU | S | 813 | 29.928 | 8.375 | 36.190 | 1.00 | 42.70 | N |
| ATOM | 2791 | CA | LEU | S | 813 | 30.620 | 8.776 | 34.969 | 1.00 | 42.21 | C |
| ATOM | 2792 | C | LEU | S | 813 | 29.711 | 9.604 | 34.057 | 1.00 | 41.46 | C |
| ATOM | 2793 | O | LEU | S | 813 | 28.492 | 9.438 | 34.062 | 1.00 | 41.23 | O |
| ATOM | 2794 | CB | LEU | S | 813 | 31.167 | 7.554 | 34.225 | 1.00 | 42.30 | C |
| ATOM | 2795 | CG | LEU | S | 813 | 32.093 | 6.644 | 35.046 | 1.00 | 42.35 | C |
| ATOM | 2796 | CD1 | LEU | S | 813 | 32.494 | 5.419 | 34.233 | 1.00 | 42.48 | C |
| ATOM | 2797 | CD2 | LEU | S | 813 | 33.322 | 7.398 | 35.527 | 1.00 | 41.80 | C |
| ATOM | 2798 | N | GLN | S | 814 | 30.326 | 10.492 | 33.283 | 1.00 | 40.74 | N |
| ATOM | 2799 | CA | GLN | S | 814 | 29.603 | 11.385 | 32.378 | 1.00 | 40.26 | C |
| ATOM | 2800 | C | GLN | S | 814 | 30.475 | 11.775 | 31.190 | 1.00 | 39.82 | C |
| ATOM | 2801 | O | GLN | S | 814 | 31.674 | 11.514 | 31.176 | 1.00 | 39.19 | O |
| ATOM | 2802 | CB | GLN | S | 814 | 29.173 | 12.649 | 33.122 | 1.00 | 40.24 | C |
| ATOM | 2803 | CG | GLN | S | 814 | 30.336 | 13.501 | 33.615 | 1.00 | 40.51 | C |
| ATOM | 2804 | CD | GLN | S | 814 | 29.879 | 14.725 | 34.406 | 1.00 | 41.88 | C |
| ATOM | 2805 | OE1 | GLN | S | 814 | 29.200 | 14.590 | 35.419 | 1.00 | 41.86 | O |
| ATOM | 2806 | NE2 | GLN | S | 814 | 30.253 | 15.919 | 33.940 | 1.00 | 40.63 | N |
| ATOM | 2807 | N | GLY | S | 815 | 29.864 | 12.416 | 30.200 | 1.00 | 39.81 | N |
| ATOM | 2808 | CA | GLY | S | 815 | 30.568 | 12.851 | 29.012 | 1.00 | 39.53 | C |
| ATOM | 2809 | C | GLY | S | 815 | 31.402 | 11.755 | 28.365 | 1.00 | 39.85 | C |
| ATOM | 2810 | O | GLY | S | 815 | 30.962 | 10.609 | 28.210 | 1.00 | 38.55 | O |
| ATOM | 2811 | N | GLU | S | 816 | 32.624 | 12.123 | 27.995 | 1.00 | 40.44 | N |
| ATOM | 2812 | CA | GLU | S | 816 | 33.553 | 11.208 | 27.352 | 1.00 | 41.24 | C |
| ATOM | 2813 | C | GLU | S | 816 | 33.744 | 9.926 | 28.154 | 1.00 | 41.73 | C |
| ATOM | 2814 | O | GLU | S | 816 | 33.895 | 8.852 | 27.577 | 1.00 | 41.11 | O |
| ATOM | 2815 | CB | GLU | S | 816 | 34.909 | 11.884 | 27.148 | 1.00 | 41.24 | C |
| ATOM | 2816 | CG | GLU | S | 816 | 35.752 | 11.238 | 26.063 | 1.00 | 42.19 | C |
| ATOM | 2817 | CD | GLU | S | 816 | 37.161 | 11.790 | 26.019 | 1.00 | 43.70 | C |

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ATOM   2818  OE1 GLU S 816      37.985  11.311  26.814  1.00 45.25           O
ATOM   2819  OE2 GLU S 816      37.447  12.696  25.201  1.00 44.50           O
ATOM   2820  N   GLU S 817      33.724  10.039  29.479  1.00 42.66           N
ATOM   2821  CA  GLU S 817      33.925   8.877  30.340  1.00 43.73           C
ATOM   2822  C   GLU S 817      32.744   7.917  30.268  1.00 44.19           C
ATOM   2823  O   GLU S 817      32.930   6.699  30.252  1.00 43.99           O
ATOM   2824  CB  GLU S 817      34.167   9.308  31.788  1.00 43.81           C
ATOM   2825  CG  GLU S 817      35.463  10.077  31.989  1.00 44.98           C
ATOM   2826  CD  GLU S 817      35.337  11.569  31.688  1.00 46.95           C
ATOM   2827  OE1 GLU S 817      34.221  12.052  31.394  1.00 48.87           O
ATOM   2828  OE2 GLU S 817      36.362  12.277  31.748  1.00 49.02           O
ATOM   2829  N   LEU S 818      31.536   8.470  30.231  1.00 44.93           N
ATOM   2830  CA  LEU S 818      30.335   7.663  30.149  1.00 45.78           C
ATOM   2831  C   LEU S 818      30.359   6.882  28.846  1.00 46.89           C
ATOM   2832  O   LEU S 818      30.163   5.663  28.833  1.00 46.50           O
ATOM   2833  CB  LEU S 818      29.077   8.537  30.219  1.00 45.65           C
ATOM   2834  CG  LEU S 818      27.741   7.788  30.147  1.00 45.58           C
ATOM   2835  CD1 LEU S 818      27.612   6.809  31.318  1.00 45.36           C
ATOM   2836  CD2 LEU S 818      26.551   8.719  30.133  1.00 43.95           C
ATOM   2837  N   LEU S 819      30.654   7.588  27.760  1.00 48.01           N
ATOM   2838  CA  LEU S 819      30.607   7.014  26.420  1.00 49.24           C
ATOM   2839  C   LEU S 819      31.559   5.829  26.247  1.00 50.32           C
ATOM   2840  O   LEU S 819      31.169   4.777  25.731  1.00 50.11           O
ATOM   2841  CB  LEU S 819      30.903   8.105  25.380  1.00 49.22           C
ATOM   2842  CG  LEU S 819      30.848   7.724  23.901  1.00 49.32           C
ATOM   2843  CD1 LEU S 819      29.495   7.178  23.497  1.00 48.73           C
ATOM   2844  CD2 LEU S 819      31.205   8.940  23.058  1.00 49.85           C
ATOM   2845  N   ARG S 820      32.801   6.005  26.684  1.00 51.33           N
ATOM   2846  CA  ARG S 820      33.807   4.966  26.550  1.00 52.53           C
ATOM   2847  C   ARG S 820      33.471   3.748  27.414  1.00 52.95           C
ATOM   2848  O   ARG S 820      33.534   2.606  26.942  1.00 53.06           O
ATOM   2849  CB  ARG S 820      35.185   5.529  26.898  1.00 52.91           C
ATOM   2850  CG  ARG S 820      35.620   6.583  25.904  1.00 54.20           C
ATOM   2851  CD  ARG S 820      37.044   7.046  26.040  1.00 55.94           C
ATOM   2852  NE  ARG S 820      37.320   8.113  25.081  1.00 58.09           N
ATOM   2853  CZ  ARG S 820      38.453   8.808  25.022  1.00 59.82           C
ATOM   2854  NH1 ARG S 820      39.448   8.555  25.867  1.00 60.28           N
ATOM   2855  NH2 ARG S 820      38.590   9.765  24.108  1.00 60.61           N
ATOM   2856  N   ALA S 821      33.106   3.994  28.670  1.00 53.36           N
ATOM   2857  CA  ALA S 821      32.698   2.920  29.561  1.00 53.67           C
ATOM   2858  C   ALA S 821      31.598   2.094  28.892  1.00 54.08           C
ATOM   2859  O   ALA S 821      31.648   0.862  28.897  1.00 54.01           O
ATOM   2860  CB  ALA S 821      32.215   3.479  30.883  1.00 53.55           C
ATOM   2861  N   LEU S 822      30.616   2.777  28.308  1.00 54.44           N
ATOM   2862  CA  LEU S 822      29.516   2.110  27.622  1.00 54.93           C
ATOM   2863  C   LEU S 822      30.007   1.342  26.398  1.00 55.41           C
ATOM   2864  O   LEU S 822      29.557   0.230  26.143  1.00 55.60           O
ATOM   2865  CB  LEU S 822      28.445   3.117  27.212  1.00 54.90           C
ATOM   2866  CG  LEU S 822      27.667   3.756  28.361  1.00 54.80           C
ATOM   2867  CD1 LEU S 822      26.531   4.601  27.801  1.00 54.39           C
ATOM   2868  CD2 LEU S 822      27.139   2.702  29.335  1.00 54.48           C
ATOM   2869  N   ASP S 823      30.911   1.949  25.634  1.00 55.82           N
ATOM   2870  CA  ASP S 823      31.525   1.282  24.492  1.00 56.04           C
ATOM   2871  C   ASP S 823      32.893   0.735  24.901  1.00 56.10           C
ATOM   2872  O   ASP S 823      33.186  -0.451  24.731  1.00 56.09           O
ATOM   2873  CB  ASP S 823      31.688   2.252  23.320  1.00 56.21           C
ATOM   2874  CG  ASP S 823      31.858   1.535  21.997  1.00 56.45           C
ATOM   2875  OD1 ASP S 823      32.245   0.351  22.028  1.00 58.65           O
ATOM   2876  OD2 ASP S 823      31.628   2.056  20.885  1.00 56.19           O
TER    2877       ASP S 823
HETATM 2878 FE   FE2 A1350      23.294  27.501  28.594  1.00 20.46          FE
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HETATM 2879  C1  OGA A1351      22.091  25.173  27.594  1.00 24.79           C
HETATM 2880  C2  OGA A1351      21.066  25.829  28.202  1.00 24.27           C
HETATM 2881  C4  OGA A1351      18.756  25.714  29.004  1.00 23.09           C
HETATM 2882  C5  OGA A1351      17.415  25.241  28.495  1.00 23.17           C
HETATM 2883  O1  OGA A1351      21.909  24.061  27.090  1.00 25.24           O
HETATM 2884  O2  OGA A1351      23.219  25.658  27.531  1.00 24.40           O
HETATM 2885  O2' OGA A1351      21.192  26.959  28.711  1.00 21.19           O
HETATM 2886  O3  OGA A1351      16.416  25.662  29.055  1.00 23.03           O
HETATM 2887  N1  OGA A1351      19.886  25.203  28.228  1.00 21.70           N
HETATM 2888  O4  OGA A1351      17.332  24.475  27.537  1.00 23.98           O
HETATM 2889  S   SO4 A1352       0.316  25.182  43.602  1.00 77.77           S
HETATM 2890  O1  SO4 A1352       1.239  25.980  44.403  1.00 77.64           O
HETATM 2891  O2  SO4 A1352       1.075  24.260  42.760  1.00 77.88           O
HETATM 2892  O3  SO4 A1352      -0.525  24.416  44.514  1.00 78.38           O
HETATM 2893  O4  SO4 A1352      -0.507  26.042  42.757  1.00 76.90           O
HETATM 2894  S   SO4 A1353       1.990  28.487  29.834  1.00 69.20           S
HETATM 2895  O1  SO4 A1353       3.243  29.065  30.309  1.00 68.34           O
HETATM 2896  O2  SO4 A1353       2.236  27.438  28.847  1.00 67.90           O
HETATM 2897  O3  SO4 A1353       1.298  27.948  31.009  1.00 70.32           O
HETATM 2898  O4  SO4 A1353       1.162  29.517  29.203  1.00 69.63           O
HETATM 2899  O   HOH H    1     35.955  31.618  40.285  1.00 80.01           O
HETATM 2900  O   HOH H    2     38.513  33.804  31.613  1.00 33.04           O
HETATM 2901  O   HOH H    3     36.648  25.786  38.779  1.00 76.96           O
HETATM 2902  O   HOH H    4     38.106  25.337  29.179  1.00 54.79           O
HETATM 2903  O   HOH H    5     34.990  30.561  34.967  1.00 30.13           O
HETATM 2904  O   HOH H    6     33.934  31.237  38.711  1.00 40.66           O
HETATM 2905  O   HOH H    7     30.766  25.787  37.613  1.00 54.75           O
HETATM 2906  O   HOH H    8     33.667  28.867  40.196  1.00 59.66           O
HETATM 2907  O   HOH H    9     28.622  27.043  37.556  1.00 57.58           O
HETATM 2908  O   HOH H   10     19.894  26.655  33.706  1.00 54.88           O
HETATM 2909  O   HOH H   11     30.052  24.213  35.628  1.00 41.23           O
HETATM 2910  O   HOH H   12     28.737  12.960  37.083  1.00 59.80           O
HETATM 2911  O   HOH H   13     35.568  13.822  23.888  1.00 38.00           O
HETATM 2912  O   HOH H   14     30.722  -1.323  21.296  1.00 48.92           O
HETATM 2913  O   HOH H   15     32.110   2.136  17.673  1.00 69.92           O
HETATM 2914  O   HOH Z    1      9.466  21.720  12.039  1.00 63.79           O
HETATM 2915  O   HOH Z    2      1.367  21.270   7.724  1.00 60.01           O
HETATM 2916  O   HOH Z    3      3.426  13.325   8.811  1.00 43.04           O
HETATM 2917  O   HOH Z    4     -0.760  13.029   7.574  1.00 47.08           O
HETATM 2918  O   HOH Z    5      2.515  19.304   5.195  1.00 46.76           O
HETATM 2919  O   HOH Z    6      4.861  33.534  13.331  1.00 75.60           O
HETATM 2920  O   HOH Z    7      1.403  29.250  13.007  1.00 46.80           O
HETATM 2921  O   HOH Z    8      1.614  32.100  13.758  1.00 66.18           O
HETATM 2922  O   HOH Z    9     12.671  34.540  13.968  1.00 43.83           O
HETATM 2923  O   HOH Z   10     11.399   2.867  17.750  1.00 68.06           O
HETATM 2924  O   HOH Z   11     -1.220  30.205  22.820  1.00 80.54           O
HETATM 2925  O   HOH Z   12      6.576  36.529  29.511  1.00 43.88           O
HETATM 2926  O   HOH Z   13      3.525  32.513  31.866  1.00 65.87           O
HETATM 2927  O   HOH Z   14      5.033  37.447  27.566  1.00 54.03           O
HETATM 2928  O   HOH Z   15     10.981  35.615  30.196  1.00 36.24           O
HETATM 2929  O   HOH Z   16     12.816  42.461  26.787  1.00 37.83           O
HETATM 2930  O   HOH Z   17     13.508  37.138  13.905  1.00 50.79           O
HETATM 2931  O   HOH Z   18     16.409   3.305  16.425  1.00 59.87           O
HETATM 2932  O   HOH Z   19     14.424   4.598  17.530  1.00 54.39           O
HETATM 2933  O   HOH Z   20     11.439   7.927  15.708  1.00 63.10           O
HETATM 2934  O   HOH Z   21     15.821  30.360  12.573  1.00 43.61           O
HETATM 2935  O   HOH Z   22     13.496  22.189   7.246  1.00 57.93           O
HETATM 2936  O   HOH Z   23     17.591  29.863   7.160  1.00 49.97           O
HETATM 2937  O   HOH Z   24     14.617  26.200  13.898  1.00 48.56           O
HETATM 2938  O   HOH Z   25     20.840  23.785   3.695  1.00 38.79           O
HETATM 2939  O   HOH Z   26     27.946  19.151   9.101  1.00 43.14           O
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|---|---|---|---|---|---|---|---|---|---|---|
| HETATM | 2940 | O | HOH | Z | 27 | 23.279 | 21.788 | 0.672 | 1.00 | 62.23 | O |
| HETATM | 2941 | O | HOH | Z | 28 | 27.443 | 22.009 | 43.177 | 1.00 | 68.81 | O |
| HETATM | 2942 | O | HOH | Z | 29 | 27.326 | 30.900 | 5.769 | 1.00 | 84.31 | O |
| HETATM | 2943 | O | HOH | Z | 30 | 16.938 | 35.662 | 41.749 | 1.00 | 51.88 | O |
| HETATM | 2944 | O | HOH | Z | 31 | 36.792 | 29.262 | 21.033 | 1.00 | 42.38 | O |
| HETATM | 2945 | O | HOH | Z | 32 | 26.719 | 37.403 | 13.167 | 1.00 | 60.20 | O |
| HETATM | 2946 | O | HOH | Z | 33 | 29.797 | 37.021 | 10.379 | 1.00 | 60.24 | O |
| HETATM | 2947 | O | HOH | Z | 34 | 28.365 | 37.713 | 15.023 | 1.00 | 68.08 | O |
| HETATM | 2948 | O | HOH | Z | 35 | 27.471 | 34.815 | 9.298 | 1.00 | 63.90 | O |
| HETATM | 2949 | O | HOH | Z | 36 | 24.262 | 32.919 | 12.792 | 1.00 | 45.02 | O |
| HETATM | 2950 | O | HOH | Z | 37 | 19.704 | 17.909 | 13.178 | 1.00 | 28.78 | O |
| HETATM | 2951 | O | HOH | Z | 38 | 22.022 | 12.870 | 8.792 | 1.00 | 48.37 | O |
| HETATM | 2952 | O | HOH | Z | 39 | 18.151 | 14.971 | 12.982 | 1.00 | 36.76 | O |
| HETATM | 2953 | O | HOH | Z | 40 | 29.160 | 5.439 | 16.977 | 1.00 | 44.05 | O |
| HETATM | 2954 | O | HOH | Z | 41 | 18.863 | 14.590 | 16.204 | 1.00 | 30.84 | O |
| HETATM | 2955 | O | HOH | Z | 42 | 12.149 | 5.293 | 13.385 | 1.00 | 72.13 | O |
| HETATM | 2956 | O | HOH | Z | 43 | 15.651 | 2.782 | 13.845 | 1.00 | 41.52 | O |
| HETATM | 2957 | O | HOH | Z | 44 | 14.014 | 7.467 | 18.234 | 1.00 | 52.22 | O |
| HETATM | 2958 | O | HOH | Z | 45 | 5.548 | 12.548 | 27.846 | 1.00 | 38.03 | O |
| HETATM | 2959 | O | HOH | Z | 46 | 12.742 | 5.782 | 36.187 | 1.00 | 51.07 | O |
| HETATM | 2960 | O | HOH | Z | 47 | 19.063 | 6.567 | 36.600 | 1.00 | 49.16 | O |
| HETATM | 2961 | O | HOH | Z | 48 | 19.545 | 2.633 | 38.104 | 1.00 | 67.28 | O |
| HETATM | 2962 | O | HOH | Z | 49 | 7.710 | 14.276 | 19.473 | 1.00 | 48.41 | O |
| HETATM | 2963 | O | HOH | Z | 50 | 15.732 | 7.234 | 38.833 | 1.00 | 54.12 | O |
| HETATM | 2964 | O | HOH | Z | 51 | 21.932 | 13.291 | 44.351 | 1.00 | 62.49 | O |
| HETATM | 2965 | O | HOH | Z | 52 | 33.998 | 44.086 | 25.334 | 1.00 | 53.56 | O |
| HETATM | 2966 | O | HOH | Z | 53 | 12.673 | 21.178 | 43.612 | 1.00 | 63.01 | O |
| HETATM | 2967 | O | HOH | Z | 54 | 8.172 | 26.738 | 44.107 | 1.00 | 61.46 | O |
| HETATM | 2968 | O | HOH | Z | 55 | 9.613 | 30.854 | 42.520 | 1.00 | 54.56 | O |
| HETATM | 2969 | O | HOH | Z | 56 | 13.563 | 35.806 | 31.131 | 1.00 | 39.09 | O |
| HETATM | 2970 | O | HOH | Z | 57 | 15.688 | 37.473 | 35.304 | 1.00 | 47.58 | O |
| HETATM | 2971 | O | HOH | Z | 58 | 7.422 | 43.868 | 25.982 | 1.00 | 75.57 | O |
| HETATM | 2972 | O | HOH | Z | 59 | 7.978 | 38.223 | 34.865 | 1.00 | 59.51 | O |
| HETATM | 2973 | O | HOH | Z | 60 | 16.338 | 30.836 | 40.223 | 1.00 | 38.80 | O |
| HETATM | 2974 | O | HOH | Z | 61 | 17.035 | 27.760 | 38.288 | 1.00 | 52.22 | O |
| HETATM | 2975 | O | HOH | Z | 62 | 22.131 | 25.023 | 41.390 | 1.00 | 55.16 | O |
| HETATM | 2976 | O | HOH | Z | 63 | 29.869 | 29.910 | 39.122 | 1.00 | 47.28 | O |
| HETATM | 2977 | O | HOH | Z | 64 | 28.353 | 24.399 | 41.766 | 1.00 | 60.35 | O |
| HETATM | 2978 | O | HOH | Z | 65 | 31.794 | 27.570 | 41.962 | 1.00 | 48.59 | O |
| HETATM | 2979 | O | HOH | Z | 66 | 28.058 | 28.695 | 48.927 | 1.00 | 65.95 | O |
| HETATM | 2980 | O | HOH | Z | 67 | 24.838 | 24.783 | 42.190 | 1.00 | 52.90 | O |
| HETATM | 2981 | O | HOH | Z | 68 | 11.541 | 32.183 | 15.082 | 1.00 | 63.99 | O |
| HETATM | 2982 | O | HOH | Z | 69 | 31.599 | 33.767 | 45.823 | 1.00 | 44.28 | O |
| HETATM | 2983 | O | HOH | Z | 70 | 24.728 | 38.721 | 49.282 | 1.00 | 48.25 | O |
| HETATM | 2984 | O | HOH | Z | 71 | 16.271 | 36.399 | 44.087 | 1.00 | 58.46 | O |
| HETATM | 2985 | O | HOH | Z | 72 | 17.845 | 37.716 | 46.244 | 1.00 | 57.93 | O |
| HETATM | 2986 | O | HOH | Z | 73 | 16.480 | 33.117 | 41.520 | 1.00 | 59.15 | O |
| HETATM | 2987 | O | HOH | Z | 74 | 40.791 | 21.415 | 26.920 | 1.00 | 58.98 | O |
| HETATM | 2988 | O | HOH | Z | 75 | 21.842 | 17.819 | 48.106 | 1.00 | 67.11 | O |
| HETATM | 2989 | O | HOH | Z | 76 | 8.791 | 17.468 | 46.626 | 1.00 | 63.28 | O |
| HETATM | 2990 | O | HOH | Z | 77 | 17.141 | 16.914 | 47.607 | 1.00 | 52.87 | O |
| HETATM | 2991 | O | HOH | Z | 78 | 21.626 | 14.804 | 40.702 | 1.00 | 53.91 | O |
| HETATM | 2992 | O | HOH | Z | 79 | 39.117 | 50.091 | 47.735 | 1.00 | 57.17 | O |
| HETATM | 2993 | O | HOH | Z | 80 | 10.617 | 19.257 | 44.587 | 1.00 | 69.00 | O |
| HETATM | 2994 | O | HOH | Z | 81 | 1.682 | 24.435 | 36.842 | 1.00 | 55.40 | O |
| HETATM | 2995 | O | HOH | Z | 82 | 4.627 | 30.781 | 36.487 | 1.00 | 53.38 | O |
| HETATM | 2996 | O | HOH | Z | 83 | 17.463 | 26.906 | 33.818 | 1.00 | 38.64 | O |
| HETATM | 2997 | O | HOH | Z | 84 | 18.429 | 25.785 | 36.464 | 1.00 | 54.65 | O |
| HETATM | 2998 | O | HOH | Z | 85 | 23.466 | 17.336 | 36.578 | 1.00 | 41.94 | O |
| HETATM | 2999 | O | HOH | Z | 86 | 26.890 | 12.949 | 30.365 | 1.00 | 49.34 | O |
| HETATM | 3000 | O | HOH | Z | 87 | 21.694 | 10.405 | 34.333 | 1.00 | 45.95 | O |

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HETATM 3001  O   HOH Z  88      20.030   9.589  36.847  1.00 52.33           O
HETATM 3002  O   HOH Z  89      18.447  -1.706  32.981  1.00 66.29           O
HETATM 3003  O   HOH Z  90      16.300  -0.205  30.017  1.00 50.70           O
HETATM 3004  O   HOH Z  91      17.950   1.645  20.589  1.00 51.55           O
HETATM 3005  O   HOH Z  92      26.301   5.439  16.918  1.00 36.67           O
HETATM 3006  O   HOH Z  93      33.944  10.218  13.383  1.00 51.60           O
HETATM 3007  O   HOH Z  94      30.893  16.371  11.174  1.00 40.00           O
HETATM 3008  O   HOH Z  95      32.606  13.689  20.709  1.00 45.01           O
HETATM 3009  O   HOH Z  96      31.860  10.158   7.765  1.00 58.55           O
HETATM 3010  O   HOH Z  97      36.957  10.422   7.614  1.00 76.91           O
HETATM 3011  O   HOH Z  98      35.951  16.836  31.735  1.00 59.28           O
HETATM 3012  O   HOH Z  99      39.867  18.412  27.150  1.00 50.38           O
HETATM 3013  O   HOH Z 100      13.436  20.952  28.355  1.00 27.89           O
HETATM 3014  O   HOH Z 101       3.992  21.265  30.540  1.00 43.76           O
HETATM 3015  O   HOH Z 102      30.735  37.910  33.103  1.00 30.45           O
HETATM 3016  O   HOH Z 103      25.986  26.303  26.047  1.00 26.08           O
HETATM 3017  O   HOH Z 104      36.837  32.025  33.001  1.00 37.86           O
HETATM 3018  O   HOH Z 105      35.845  25.360  27.653  1.00 33.53           O
HETATM 3019  O   HOH Z 106      31.874  20.474  33.040  1.00 55.47           O
HETATM 3020  O   HOH Z 107      36.793  26.619  20.918  1.00 34.57           O
HETATM 3021  O   HOH Z 108      17.114  16.909  17.862  1.00 35.83           O
HETATM 3022  O   HOH Z 109       9.968  13.510  19.464  1.00 37.10           O
HETATM 3023  O   HOH Z 110       5.274  16.717  22.023  1.00 44.26           O
HETATM 3024  O   HOH Z 111       7.041  16.862  20.149  1.00 37.71           O
HETATM 3025  O   HOH Z 112       6.517  22.763  22.963  1.00 38.94           O
HETATM 3026  O   HOH Z 113      29.471  38.812  26.249  1.00 22.19           O
HETATM 3027  O   HOH Z 114      32.253  43.121  24.229  1.00 53.95           O
HETATM 3028  O   HOH Z 115      28.797  40.227  16.136  1.00 64.15           O
HETATM 3029  O   HOH Z 116      30.645  39.042  18.925  1.00 33.21           O
HETATM 3030  O   HOH Z 117      25.466  42.302  17.883  1.00 64.00           O
HETATM 3031  O   HOH Z 118      27.698  44.486  31.068  1.00 26.13           O
HETATM 3032  O   HOH Z 119      30.274  44.879  25.031  1.00 38.32           O
HETATM 3033  O   HOH Z 120      27.635  48.525  29.776  1.00 35.59           O
HETATM 3034  O   HOH Z 121      25.933  50.527  30.463  1.00 35.79           O
HETATM 3035  O   HOH Z 122      26.614  31.094  38.158  1.00 32.11           O
HETATM 3036  O   HOH Z 123      29.486  36.934  35.226  1.00 27.40           O
HETATM 3037  O   HOH Z 124      30.510  30.229  36.300  1.00 31.99           O
HETATM 3038  O   HOH Z 125      19.859  31.575  33.786  1.00 31.77           O
HETATM 3039  O   HOH Z 126      18.490  38.301  36.415  1.00 43.54           O
HETATM 3040  O   HOH Z 127      19.538  36.155  33.217  1.00 30.91           O
HETATM 3041  O   HOH Z 128      25.386  44.358  40.124  1.00 54.33           O
HETATM 3042  O   HOH Z 129      21.227  42.704  39.938  1.00 38.88           O
HETATM 3043  O   HOH Z 130      17.603  37.763  31.961  1.00 35.39           O
HETATM 3044  O   HOH Z 131       9.290  41.007  35.589  1.00 51.53           O
HETATM 3045  O   HOH Z 132       9.348  43.374  27.752  1.00 61.17           O
HETATM 3046  O   HOH Z 133      15.089  37.816  32.481  1.00 32.05           O
HETATM 3047  O   HOH Z 134      10.824  48.278  31.295  1.00 52.52           O
HETATM 3048  O   HOH Z 135      15.691  44.668  34.824  1.00 31.47           O
HETATM 3049  O   HOH Z 136      15.962  46.870  38.981  1.00 51.42           O
HETATM 3050  O   HOH Z 137      13.481  51.613  32.894  1.00 45.77           O
HETATM 3051  O   HOH Z 138      14.202  48.658  24.558  1.00 43.59           O
HETATM 3052  O   HOH Z 139      16.193  44.497  37.574  1.00 58.87           O
HETATM 3053  O   HOH Z 140      15.573  46.265  24.419  1.00 39.51           O
HETATM 3054  O   HOH Z 141      18.684  55.873  28.304  1.00 58.28           O
HETATM 3055  O   HOH Z 142      14.817  55.477  27.388  1.00 52.87           O
HETATM 3056  O   HOH Z 143      15.284  50.258  22.000  1.00 32.96           O
HETATM 3057  O   HOH Z 144      23.651  46.151  19.718  1.00 33.04           O
HETATM 3058  O   HOH Z 145      16.751  46.565  21.800  1.00 33.97           O
HETATM 3059  O   HOH Z 146      12.595  29.171  13.536  1.00 39.79           O
HETATM 3060  O   HOH Z 147      10.812  19.188  14.084  1.00 50.88           O
HETATM 3061  O   HOH Z 148      11.495  21.508  13.792  1.00 44.23           O
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HETATM 3062  O   HOH Z 149      14.521  18.471  12.156  1.00 37.16           O
HETATM 3063  O   HOH Z 150      33.566  26.082  16.801  1.00 38.34           O
HETATM 3064  O   HOH Z 151      27.798  27.494  24.390  1.00 25.11           O
HETATM 3065  O   HOH Z 152      30.253  36.176  26.688  1.00 27.79           O
HETATM 3066  O   HOH Z 153      32.762  34.069  19.065  1.00 47.61           O
HETATM 3067  O   HOH Z 154      27.363  30.094  25.612  1.00 23.74           O
HETATM 3068  O   HOH Z 155      16.282  36.168  29.566  1.00 33.13           O
HETATM 3069  O   HOH Z 156      13.289  26.522  28.472  1.00 47.17           O
HETATM 3070  O   HOH Z 157       7.556  30.888  24.716  1.00 44.35           O
HETATM 3071  O   HOH Z 158       7.790  30.392  27.265  1.00 37.71           O
HETATM 3072  O   HOH Z 159       3.910  21.360  21.198  1.00 60.23           O
HETATM 3073  O   HOH Z 160       6.411  23.837  25.422  1.00 40.51           O
HETATM 3074  O   HOH Z 161       3.001  17.561  27.759  1.00 55.61           O
HETATM 3075  O   HOH Z 162       5.352  18.754  24.064  1.00 42.17           O
HETATM 3076  O   HOH Z 163      40.897  21.985  24.633  1.00 54.83           O
HETATM 3077  O   HOH Z 164      42.626  37.977  17.732  1.00 71.69           O
HETATM 3078  O   HOH Z 165      42.463  44.114  19.559  1.00 54.59           O
HETATM 3079  O   HOH Z 166      33.754  36.855  19.984  1.00 36.17           O
HETATM 3080  O   HOH Z 167      33.194  39.271  33.406  1.00 28.26           O
HETATM 3081  O   HOH Z 168      37.482  29.751  37.743  1.00 57.74           O
HETATM 3082  O   HOH Z 169      38.789  34.566  42.752  1.00 40.46           O
HETATM 3083  O   HOH Z 170      32.020  40.390  44.008  1.00 38.46           O
HETATM 3084  O   HOH Z 171      31.865  44.151  45.174  1.00 45.64           O
HETATM 3085  O   HOH Z 172      41.427  43.475  51.164  1.00 50.64           O
HETATM 3086  O   HOH Z 173      38.498  47.344  48.085  1.00 60.19           O
HETATM 3087  O   HOH Z 174      35.239  52.784  45.826  1.00 54.63           O
HETATM 3088  O   HOH Z 175      32.343  51.933  45.286  1.00 58.03           O
HETATM 3089  O   HOH Z 176      39.267  57.239  41.745  1.00 26.45           O
HETATM 3090  O   HOH Z 177      32.755  59.287  44.804  1.00 60.46           O
HETATM 3091  O   HOH Z 178      46.839  53.182  31.757  1.00 31.38           O
HETATM 3092  O   HOH Z 179      37.840  55.111  29.241  1.00 44.20           O
CONECT 1478 2878
CONECT 1498 2878
CONECT 2167 2878
CONECT 2878 2885 2884 1478 2167 1498
CONECT 2879 2880 2883 2884
CONECT 2880 2879 2885 2887
CONECT 2881 2882 2887
CONECT 2882 2881 2886 2888
CONECT 2883 2879
CONECT 2884 2879 2878
CONECT 2885 2880 2878
CONECT 2886 2882
CONECT 2887 2880 2881
CONECT 2888 2882
CONECT 2889 2890 2891 2892 2893
CONECT 2890 2889
CONECT 2891 2889
CONECT 2892 2889
CONECT 2893 2889
CONECT 2894 2895 2896 2897 2898
CONECT 2895 2894
CONECT 2896 2894
CONECT 2897 2894
CONECT 2898 2894
MASTER      455    0    4   15   20    0    7    6 3090    2   24   31
END
```

Structure 2

Below are the coordinates for structure 2 (the 2.25 Å structure of FIH:Fe(II):2OG:CAD):

```
HEADER    TRANSCRIPTION ACTIVATOR/INHIBITOR       12-AUG-02   1H2L
TITLE     FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE    2 FRAGMENT PEPTIDE
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND   3 CHAIN: A;
COMPND   4 ENGINEERED: YES;
COMPND   5 MOL_ID: 2;
COMPND   6 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND   7 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND   8  MEMBER OF PAS PROTEIN 1;
COMPND   9 CHAIN: S;
COMPND  10 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND  11  RESIDUES 786-826
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   3 ORGANISM_COMMON: HUMAN;
SOURCE   4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE   5 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE   6 EXPRESSION_SYSTEM_PLASMID: PET28A(+);
SOURCE   7 MOL_ID: 2;
SOURCE   8 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   9 ORGANISM_COMMON: HUMAN;
SOURCE  10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE  11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE  12 EXPRESSION_SYSTEM_PLASMID: PGEX-GP-1
KEYWDS    FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
KEYWDS   2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
EXPDTA    X-RAY DIFFRACTION
AUTHOR    J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,I.SCHLEMMINGER,
AUTHOR   2 J.F.SEIBEL,C.J.SCHOFIELD
REVDAT   1   04-SEP-02 1H2L    0
JRNL        AUTH   J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,
JRNL        AUTH 2 I.SCHLEMMINGER,J.F.SEIBEL,C.J.SCHOFIELD
JRNL        TITL   FIH:HIF-FRAGMENT COMPLEXES
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK   2
REMARK   2 RESOLUTION. 2.25 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.0
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) :   2.25
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) :  38.00
REMARK   3   DATA CUTOFF            (SIGMA(F)) : NONE
REMARK   3   COMPLETENESS FOR RANGE        (%) :  99.98
REMARK   3   NUMBER OF REFLECTIONS             :  25127
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD           : THROUGHOUT
```

```
REMARK   3   FREE R VALUE TEST SET SELECTION   : RANDOM
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.18514
REMARK   3   R VALUE           (WORKING SET) :  0.18253
REMARK   3   FREE R VALUE                    :  0.21738
REMARK   3   FREE R VALUE TEST SET SIZE   (%) :  7.7
REMARK   3   FREE R VALUE TEST SET COUNT      :  2104
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           :       20
REMARK   3   BIN RESOLUTION RANGE HIGH           :    2.250
REMARK   3   BIN RESOLUTION RANGE LOW            :    2.308
REMARK   3   REFLECTION IN BIN     (WORKING SET) :     1783
REMARK   3   BIN R VALUE           (WORKING SET) :    0.194
REMARK   3   BIN FREE R VALUE SET COUNT          :      170
REMARK   3   BIN FREE R VALUE                    :    0.228
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 2863
REMARK   3   NUCLEIC ACID ATOMS       : 0
REMARK   3   HETEROGEN ATOMS          : 21
REMARK   3   SOLVENT ATOMS            : 139
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) :  27.234
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :    -0.40
REMARK   3    B22 (A**2) :    -0.40
REMARK   3    B33 (A**2) :     0.80
REMARK   3    B12 (A**2) :     0.00
REMARK   3    B13 (A**2) :     0.00
REMARK   3    B23 (A**2) :     0.00
REMARK   3
REMARK   3 ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3  ESU BASED ON R VALUE                                    (A): 0.203
REMARK   3  ESU BASED ON FREE R VALUE                               (A): 0.174
REMARK   3  ESU BASED ON MAXIMUM LIKELIHOOD                         (A): 0.165
REMARK   3  ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2): 6.444
REMARK   3
REMARK   3 CORRELATION COEFFICIENTS.
REMARK   3   CORRELATION COEFFICIENT FO-FC      :   0.956
REMARK   3   CORRELATION COEFFICIENT FO-FC FREE :   0.939
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES     COUNT     RMS     WEIGHT
REMARK   3   BOND LENGTHS REFINED           (A):  2961 ; 0.013 ; 0.021
REMARK   3   BOND LENGTHS REFINED           (A):  2961 ; 0.013 ; 0.021
REMARK   3   BOND LENGTHS OTHERS            (A):  2554 ; 0.001 ; 0.020
REMARK   3   BOND ANGLES REFINED       (DEGREES):  4026 ; 1.404 ; 1.949
REMARK   3   BOND ANGLES OTHERS        (DEGREES):  5966 ; 0.727 ; 3.000
REMARK   3   TORSION ANGLES, PERIOD 1  (DEGREES):   350 ; 4.037 ; 3.000
REMARK   3   TORSION ANGLES, PERIOD 3  (DEGREES):   515 ;18.189 ;15.000
REMARK   3   CHIRAL-CENTER RESTRAINTS     (A**3):   413 ; 0.085 ; 0.200
REMARK   3   GENERAL PLANES REFINED         (A):  3315 ; 0.005 ; 0.020
REMARK   3   GENERAL PLANES OTHERS          (A):   602 ; 0.002 ; 0.020
REMARK   3   NON-BONDED CONTACTS REFINED    (A):   693 ; 0.221 ; 0.300
REMARK   3   NON-BONDED CONTACTS OTHERS     (A):  2483 ; 0.204 ; 0.300
REMARK   3   H-BOND (X...Y) REFINED         (A):   208 ; 0.156 ; 0.500
REMARK   3   SYMMETRY VDW REFINED           (A):    16 ; 0.256 ; 0.300
REMARK   3   SYMMETRY VDW OTHERS            (A):    63 ; 0.259 ; 0.300
REMARK   3   SYMMETRY H-BOND REFINED        (A):    10 ; 0.200 ; 0.500
REMARK   3
```

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REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS. COUNT  RMS   WEIGHT
REMARK   3   MAIN-CHAIN BOND REFINED   (A**2):  1767 ; 0.649 ; 1.500
REMARK   3   MAIN-CHAIN ANGLE REFINED  (A**2):  2847 ; 1.227 ; 2.000
REMARK   3   SIDE-CHAIN BOND REFINED   (A**2):  1194 ; 1.887 ; 3.000
REMARK   3   SIDE-CHAIN ANGLE REFINED  (A**2):  1179 ; 3.111 ; 4.500
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF NCS GROUPS : NULL
REMARK   3
REMARK   3  TLS DETAILS
REMARK   3   NUMBER OF TLS GROUPS  :    1
REMARK   3
REMARK   3   TLS GROUP :     1
REMARK   3    NUMBER OF COMPONENTS GROUP :    2
REMARK   3    COMPONENTS        C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :   A    15        A   451
REMARK   3    RESIDUE RANGE :   S   795        S   822
REMARK   3    ORIGIN FOR THE GROUP (A):  22.2240  27.6230  28.5830
REMARK   3    T TENSOR
REMARK   3      T11:   0.1744 T22:   0.0216
REMARK   3      T33:   0.0949 T12:  -0.0059
REMARK   3      T13:  -0.0546 T23:   0.0427
REMARK   3    L TENSOR
REMARK   3      L11:   1.1183 L22:   2.4664
REMARK   3      L33:   1.3415 L12:   0.7934
REMARK   3      L13:   0.5409 L23:   1.2249
REMARK   3    S TENSOR
REMARK   3      S11:   0.0358 S12:  -0.1772 S13:  -0.0521
REMARK   3      S21:   0.1763 S22:   0.0025 S23:   0.1089
REMARK   3      S31:   0.2114 S32:  -0.0339 S33:  -0.0383
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED : BABINET MODEL WITH MASK
REMARK   3   PARAMETERS FOR MASK CALCULATION
REMARK   3   VDW PROBE RADIUS    :  1.40
REMARK   3   ION PROBE RADIUS    :  0.80
REMARK   3   SHRINKAGE RADIUS    :  0.80
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: HYDROGENS HAVE BEEN ADDED IN THE
REMARK   3   RIDING POSITIONS
REMARK   4
REMARK   4 1H2L COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI  ON 12-AUG-2002.
REMARK 100 THE EBI ID CODE IS EBI-11172.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : 15-MAY-2002
REMARK 200  TEMPERATURE           (KELVIN) : 100
REMARK 200  PH                             : 7.5
REMARK 200  NUMBER OF CRYSTALS USED        : 1
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : Y
REMARK 200  RADIATION SOURCE               : SRS BEAMLINE PX14.2
REMARK 200  BEAMLINE                       : PX14.2
REMARK 200  X-RAY GENERATOR MODEL          : NULL
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M
REMARK 200  WAVELENGTH OR RANGE        (A) : 0.983
REMARK 200  MONOCHROMATOR                  : NULL
REMARK 200  OPTICS                         : NULL
```

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REMARK 200
REMARK 200  DETECTOR TYPE                          : CCD
REMARK 200  DETECTOR MANUFACTURER                  : ADSC
REMARK 200  INTENSITY-INTEGRATION SOFTWARE         : MOSFLM
REMARK 200  DATA SCALING SOFTWARE                  : SCALA
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS           : 27294
REMARK 200  RESOLUTION RANGE HIGH       (A)        : 2.25
REMARK 200  RESOLUTION RANGE LOW        (A)        : 38.63
REMARK 200  REJECTION CRITERIA  (SIGMA(I))         : NONE
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE      (%)        : 100.0
REMARK 200  DATA REDUNDANCY                        : 7.0
REMARK 200  R MERGE                     (I)        : 0.058
REMARK 200  R SYM                       (I)        : NULL
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET          : 9.7
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.25
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.37
REMARK 200  COMPLETENESS FOR SHELL      (%)        : 100.0
REMARK 200  DATA REDUNDANCY IN SHELL               : 7.2
REMARK 200  R MERGE FOR SHELL           (I)        : 0.307
REMARK 200  R SYM FOR SHELL             (I)        : NULL
REMARK 200  <I/SIGMA(I)> FOR SHELL                 : 2.5
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: NULL
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 63
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE, 4% PEG400,
REMARK 280  0.1M HEPES PH7.5, ARGON ATMOSPHERE, 11MG/ML PROTEIN WITH
REMARK 280  1MM FE(II), 2.5MM AKG AND 2.5MM PEPTIDE
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
REMARK 290
REMARK 290       SYMOP   SYMMETRY
REMARK 290      NNNMMM   OPERATOR
REMARK 290        1555   X,Y,Z
REMARK 290        2555   -X,-Y,1/2+Z
REMARK 290        3555   1/2-Y,1/2+X,1/4+Z
REMARK 290        4555   1/2+Y,1/2-X,3/4+Z
REMARK 290        5555   1/2-X,1/2+Y,1/4-Z
REMARK 290        6555   1/2+X,1/2-Y,3/4-Z
REMARK 290        7555   Y,X,-Z
REMARK 290        8555   -Y,-X,1/2-Z
REMARK 290
REMARK 290      WHERE NNN -> OPERATOR NUMBER
REMARK 290            MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
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```
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000       73.95700
REMARK 290   SMTRY1   3  0.000000 -1.000000  0.000000       43.13200
REMARK 290   SMTRY2   3  1.000000  0.000000  0.000000       43.13200
REMARK 290   SMTRY3   3  0.000000  0.000000  1.000000       36.97850
REMARK 290   SMTRY1   4  0.000000  1.000000  0.000000       43.13200
REMARK 290   SMTRY2   4 -1.000000  0.000000  0.000000       43.13200
REMARK 290   SMTRY3   4  0.000000  0.000000  1.000000      110.93550
REMARK 290   SMTRY1   5 -1.000000  0.000000  0.000000       43.13200
REMARK 290   SMTRY2   5  0.000000  1.000000  0.000000       43.13200
REMARK 290   SMTRY3   5  0.000000  0.000000 -1.000000       36.97850
REMARK 290   SMTRY1   6  1.000000  0.000000  0.000000       43.13200
REMARK 290   SMTRY2   6  0.000000 -1.000000  0.000000       43.13200
REMARK 290   SMTRY3   6  0.000000  0.000000 -1.000000      110.93550
REMARK 290   SMTRY1   7  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY2   7  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY3   7  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   8  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY2   8 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY3   8  0.000000  0.000000 -1.000000       73.95700
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF   2 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 300
REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC
REMARK 300
REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S
REMARK 300 PRODUCES A TETRAMER.
REMARK 300
REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE
REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT
REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE
REMARK 300 HOMODIMER OF CHAIN A
REMARK 300
REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS
REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH
REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
REMARK 300 THE CHAIN IN THE COMPLEX IS     2141.3 ANGSTROM**2
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE:  1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
```

```
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 350   BIOMT1   2  0.000000 -1.000000  0.000000       86.26400
REMARK 350   BIOMT2   2 -1.000000  0.000000  0.000000       86.26400
REMARK 350   BIOMT3   2  0.000000  0.000000 -1.000000       73.95700
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465     MET A     1
REMARK 465     ALA A     2
REMARK 465     ALA A     3
REMARK 465     THR A     4
REMARK 465     ALA A     5
REMARK 465     ALA A     6
REMARK 465     GLU A     7
REMARK 465     ALA A     8
REMARK 465     VAL A     9
REMARK 465     ALA A    10
REMARK 465     SER A    11
REMARK 465     GLY A    12
REMARK 465     SER A    13
REMARK 465     GLY A    14
REMARK 465     LYS A   304
REMARK 465     ARG A   305
REMARK 465     ILE A   306
REMARK 465     SER S   786
REMARK 465     MET S   787
REMARK 465     ASP S   788
REMARK 465     GLU S   789
REMARK 465     SER S   790
REMARK 465     GLY S   791
REMARK 465     LEU S   792
REMARK 465     PRO S   793
REMARK 465     GLN S   794
REMARK 465     GLN S   807
REMARK 465     GLY S   808
REMARK 465     SER S   809
REMARK 465     ARG S   810
REMARK 465     ASN S   811
REMARK 465     LEU S   812
REMARK 465     ASP S   823
REMARK 465     GLN S   824
REMARK 465     VAL S   825
REMARK 465     ASN S   826
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470   M RES CSSEQI  ATOMS
REMARK 470     GLU A  15    CG   CD   OE1  OE2
REMARK 470     GLU A  29    CG   CD   OE1  OE2
REMARK 470     ASN A  87    CG   OD1  ND2
REMARK 470     LYS A 106    CD   CE   NZ
REMARK 470     ARG A 117    CG   CD   NE   CZ   NH1  NH2
REMARK 470     GLN A 133    CG   CD   OE1  NE2
REMARK 470     GLN A 136    CG   CD   OE1  NE2
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REMARK 470     GLN A 137    CG   CD   OE1  NE2
REMARK 470     ARG A 156    CG   CD   NE   CZ   NH1  NH2
REMARK 470     LYS A 157    CD   CE   NZ
REMARK 470     LYS A 311    CG   CD   CE   NZ
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 500 NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,1X,2(A4,A1,3X),12X,F5.3)
REMARK 500
REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1   RES CSSEQI ATM2   DEVIATION
REMARK 500    MET A 343  SD     MET A 343  CE      -0.243
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500  ATM1  RES C  SSEQI   ATM2  RES C  SSEQI           DISTANCE
REMARK 500
REMARK 500   O    ALA A   300     OH   TYR S   798               2.18
REMARK 525
REMARK 525 SOLVENT
REMARK 525
REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
REMARK 525 ASSOCIATED WITH:
REMARK 525   PROTEIN CHAIN  SOLVENT CHAIN
REMARK 525     A              Z
REMARK 525     S              H
REMARK 600
REMARK 600 HETEROGEN
REMARK 600
REMARK 600 FOR METAL ATOM FE   FE2 A1350  THE COORDINATION ANGLES ARE:
REMARK 600  1 HIS   199A  NE2
REMARK 600  2 ASP   201A  OD2       103.4
REMARK 600  3 HIS   279A  NE2        83.1  86.0
REMARK 600  4 AKG  1351A  O1        168.9  87.6  98.2
REMARK 600  5 AKG  1351A  O5         87.0 169.4  97.2  81.9
REMARK 600                            1     2     3     4
REMARK 700
REMARK 700 SHEET
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
REMARK 700 TWO SHEETS ARE DEFINED.
REMARK 800
REMARK 800 SITE
REMARK 800 SITE_IDENTIFIER: FE1
REMARK 800 SITE_DESCRIPTION: FE BINDING SITE FOR CHAIN A
REMARK 800
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REMARK 800 SITE_IDENTIFIER: AKG
REMARK 800 SITE_DESCRIPTION: AKG BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: SO1
REMARK 800 SITE_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: SO2
REMARK 800 SITE_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1D7G   RELATED DB: PDB
REMARK 900  A MODEL FOR THE COMPLEX BETWEEN THE
REMARK 900  HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS
REMARK 900   CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE
REMARK 900 RELATED ID: 1H2K   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2M   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2N   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1L8C   RELATED DB: PDB
REMARK 900  STRUCTURAL BASIS FOR HIF-1ALPHA/CBP
REMARK 900  RECOGNITION IN THECELLULAR HYPOXIC RESPONSE
REMARK 900 RELATED ID: 1LM8   RELATED DB: PDB
REMARK 900  STRUCTURE OF A HIF-1A-PVHL-ELONGINB-
REMARK 900  ELONGINC COMPLEX
REMARK 900 RELATED ID: 1LQB   RELATED DB: PDB
REMARK 900  CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1
REMARK 900  ALPHA PEPTIDEBOUND TO THE PVHL/ELONGIN-C/
REMARK 900  ELONGIN-B COMPLEX
DBREF  1H2L A    1   349  SWS    Q969Q7   Q969Q7            1    349
DBREF  1H2L S  786   826  SWS    Q16665   HIFA_HUMAN      786    826
SEQRES   1 A  349  MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
SEQRES   2 A  349  GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEQRES   3 A  349  TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
SEQRES   4 A  349  ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
SEQRES   5 A  349  GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
SEQRES   6 A  349  ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
SEQRES   7 A  349  GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
SEQRES   8 A  349  VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
SEQRES   9 A  349  GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
SEQRES  10 A  349  SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
SEQRES  11 A  349  LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
SEQRES  12 A  349  LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
SEQRES  13 A  349  LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP
SEQRES  14 A  349  ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
SEQRES  15 A  349  THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEQRES  16 A  349  THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA
SEQRES  17 A  349  GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
SEQRES  18 A  349  ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
SEQRES  19 A  349  PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
SEQRES  20 A  349  ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY
SEQRES  21 A  349  TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE
SEQRES  22 A  349  PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN
SEQRES  23 A  349  GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY
SEQRES  24 A  349  ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA
SEQRES  25 A  349  HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET
SEQRES  26 A  349  LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
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SEQRES  27 A  349  LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
SEQRES   1 S   41  SER MET ASP GLU SER GLY LEU PRO GLN LEU THR SER TYR
SEQRES   2 S   41  ASP CYS GLU VAL ASN ALA PRO ILE GLN GLY SER ARG ASN
SEQRES   3 S   41  LEU LEU GLN GLY GLU GLU LEU LEU ARG ALA LEU ASP GLN
SEQRES   4 S   41  VAL ASN
HET    FE2  A1350       1
HET    AKG  A1351      10
HET    SO4  A1352       5
HET    SO4  A1353       5
HETNAM     FE2 FE (II) ION
HETNAM     AKG 2-OXYGLUTARIC ACID
HETNAM     SO4 SULFATE ION
FORMUL   3  FE2     FE1 2+
FORMUL   4  AKG     C5 H6 O5
FORMUL   5  SO4     2(O4 S1 2-)
FORMUL   6  HOH    *139(H2 O1)
HELIX    1   1 ASP A   28  LEU A   32  5                                    5
HELIX    2   2 ASP A   49  ASN A   58  1                                   10
HELIX    3   3 VAL A   70  TRP A   76  5                                    7
HELIX    4   4 ASP A   77  ILE A   85  1                                    9
HELIX    5   5 ASP A  104  PHE A  111  5                                    8
HELIX    6   6 LYS A  124  ARG A  138  1                                   15
HELIX    7   7 GLY A  155  GLY A  164  1                                   10
HELIX    8   8 ASN A  166  GLY A  178  1                                   13
HELIX    9   9 PRO A  220  ASP A  222  5                                    3
HELIX   10  10 GLN A  223  TYR A  228  1                                    6
HELIX   11  11 PHE A  252  VAL A  258  5                                    7
HELIX   12  12 LYS A  311  GLY A  331  1                                   21
HELIX   13  13 ASN A  332  GLN A  334  5                                    3
HELIX   14  14 GLU A  335  LYS A  345  1                                   11
HELIX   15  15 GLN S  814  LEU S  822  1                                    9
SHEET    1  AA 5 THR A  39  PRO A  41  0
SHEET    2  AA 5 GLY A 260  VAL A 265  1  O  GLY A 260   N  ARG A  40
SHEET    3  AA 5 LYS A 214  PHE A 219 -1  O  LYS A 214   N  VAL A 265
SHEET    4  AA 5 TRP A 278  SER A 283 -1  O  TRP A 278   N  PHE A 219
SHEET    5  AA 5 VAL A 195  HIS A 199 -1  O  THR A 196   N  ILE A 281
SHEET    1  AB 6 ARG A  44  LEU A  45  0
SHEET    2  AB 6 VAL A  62  LEU A  64  1  O  VAL A  63   N  LEU A  45
SHEET    3  AB 6 VAL A 270  ILE A 273 -1  O  VAL A 270   N  LEU A  64
SHEET    4  AB 6 GLN A 204  LYS A 211 -1  O  ASN A 205   N  ILE A 273
SHEET    5  AB 6 THR A 290  TYR A 297 -1  O  ILE A 291   N  ILE A 210
SHEET    6  AB 6 LEU A 182  SER A 184 -1  N  THR A 183   O  TRP A 296
SHEET    1  AC 9 ARG A  44  LEU A  45  0
SHEET    2  AC 9 VAL A  62  LEU A  64  1  O  VAL A  63   N  LEU A  45
SHEET    3  AC 9 VAL A 270  ILE A 273 -1  O  VAL A 270   N  LEU A  64
SHEET    4  AC 9 GLN A 204  LYS A 211 -1  O  ASN A 205   N  ILE A 273
SHEET    5  AC 9 THR A 290  TYR A 297 -1  O  ILE A 291   N  ILE A 210
SHEET    6  AC 9 LEU A 186  GLY A 190 -1  O  LEU A 186   N  ASN A 294
SHEET    7  AC 9 ARG A 143  THR A 149 -1  O  LEU A 146   N  ILE A 189
SHEET    8  AC 9 PHE A  90  ALA A  95 -1  O  SER A  91   N  GLN A 147
SHEET    9  AC 9 SER A 118  MET A 123 -1  O  ASN A 119   N  SER A  94
LINK         FE   FE2 A1350                 NE2 HIS A 199     1555   1555
LINK         FE   FE2 A1350                 OD2 ASP A 201     1555   1555
LINK         FE   FE2 A1350                 NE2 HIS A 279     1555   1555
LINK         FE   FE2 A1350                 O1  AKG A1351     1555   1555
LINK         FE   FE2 A1350                 O5  AKG A1351     1555   1555
CISPEP   1 TYR A  308    PRO A  309          0         1.27
SITE     1 FE1  3 HIS A 199  ASP A 201  HIS A 279
SITE     1 AKG 12 TYR A 145  THR A 196  HIS A 199  ASP A 201
SITE     2 AKG 12 ASN A 205  PHE A 207  LYS A 214  HIS A 279
SITE     3 AKG 12 ILE A 281  ASN A 294  TRP A 296  HOH Z  65
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SITE     1 SO1  4 ARG A 138  GLY A 140  GLU A 141  GLU A 142
SITE     1 SO2  5 ARG A 143  GLU A 192  GLY A 193  LEU A 285
SITE     2 SO2  5 ASN A 286
CRYST1   86.264   86.264  147.914  90.00  90.00  90.00 P 41 21 2      8
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.011592  0.000000  0.000000        0.00000
SCALE2      0.000000  0.011592  0.000000        0.00000
SCALE3      0.000000  0.000000  0.006761        0.00000
ATOM      1  N   GLU A  15       8.505  32.866   9.893  1.00 61.72           N
ATOM      2  CA  GLU A  15       7.173  32.223   9.682  1.00 61.95           C
ATOM      3  C   GLU A  15       7.251  30.749  10.070  1.00 61.54           C
ATOM      4  O   GLU A  15       8.109  30.026   9.581  1.00 61.66           O
ATOM      5  CB  GLU A  15       6.724  32.375   8.234  1.00 62.08           C
ATOM      6  N   PRO A  16       6.353  30.305  10.941  1.00 61.24           N
ATOM      7  CA  PRO A  16       6.386  28.928  11.455  1.00 60.97           C
ATOM      8  C   PRO A  16       6.342  27.853  10.368  1.00 60.27           C
ATOM      9  O   PRO A  16       5.494  27.879   9.479  1.00 60.01           O
ATOM     10  CB  PRO A  16       5.134  28.849  12.333  1.00 61.10           C
ATOM     11  CG  PRO A  16       4.790  30.262  12.653  1.00 61.53           C
ATOM     12  CD  PRO A  16       5.228  31.079  11.488  1.00 61.35           C
ATOM     13  N   ARG A  17       7.256  26.900  10.464  1.00 59.45           N
ATOM     14  CA  ARG A  17       7.348  25.820   9.494  1.00 59.05           C
ATOM     15  C   ARG A  17       6.083  24.971   9.478  1.00 57.86           C
ATOM     16  O   ARG A  17       5.312  24.963  10.437  1.00 57.86           O
ATOM     17  CB  ARG A  17       8.541  24.913   9.827  1.00 59.53           C
ATOM     18  CG  ARG A  17       9.906  25.621   9.859  1.00 60.69           C
ATOM     19  CD  ARG A  17      11.080  24.696  10.194  1.00 62.32           C
ATOM     20  NE  ARG A  17      11.040  24.185  11.567  1.00 63.73           N
ATOM     21  CZ  ARG A  17      11.464  24.852  12.649  1.00 65.28           C
ATOM     22  NH1 ARG A  17      11.962  26.085  12.544  1.00 65.01           N
ATOM     23  NH2 ARG A  17      11.385  24.282  13.848  1.00 65.09           N
ATOM     24  N   GLU A  18       5.878  24.254   8.382  1.00 56.26           N
ATOM     25  CA  GLU A  18       4.749  23.351   8.273  1.00 55.12           C
ATOM     26  C   GLU A  18       5.222  21.931   8.587  1.00 53.54           C
ATOM     27  O   GLU A  18       6.214  21.468   8.031  1.00 52.86           O
ATOM     28  CB  GLU A  18       4.150  23.406   6.867  1.00 55.33           C
ATOM     29  CG  GLU A  18       3.482  24.731   6.519  1.00 56.39           C
ATOM     30  CD  GLU A  18       2.100  24.904   7.137  1.00 57.19           C
ATOM     31  OE1 GLU A  18       1.559  23.935   7.718  1.00 56.35           O
ATOM     32  OE2 GLU A  18       1.548  26.023   7.028  1.00 58.12           O
ATOM     33  N   GLU A  19       4.526  21.260   9.501  1.00 51.73           N
ATOM     34  CA  GLU A  19       4.823  19.867   9.816  1.00 50.56           C
ATOM     35  C   GLU A  19       4.409  18.944   8.663  1.00 48.36           C
ATOM     36  O   GLU A  19       3.312  19.066   8.102  1.00 47.54           O
ATOM     37  CB  GLU A  19       4.115  19.422  11.100  1.00 51.05           C
ATOM     38  CG  GLU A  19       4.577  20.139  12.360  1.00 53.53           C
ATOM     39  CD  GLU A  19       4.363  19.323  13.638  1.00 57.67           C
ATOM     40  OE1 GLU A  19       3.906  18.146  13.561  1.00 59.24           O
ATOM     41  OE2 GLU A  19       4.663  19.864  14.735  1.00 59.50           O
ATOM     42  N   ALA A  20       5.314  18.035   8.320  1.00 46.04           N
ATOM     43  CA  ALA A  20       5.100  17.030   7.283  1.00 44.66           C
ATOM     44  C   ALA A  20       3.741  16.365   7.394  1.00 42.92           C
ATOM     45  O   ALA A  20       3.230  16.154   8.491  1.00 42.14           O
ATOM     46  CB  ALA A  20       6.182  15.965   7.360  1.00 44.46           C
ATOM     47  N   GLY A  21       3.173  16.025   6.247  1.00 41.16           N
ATOM     48  CA  GLY A  21       1.897  15.341   6.215  1.00 40.22           C
ATOM     49  C   GLY A  21       0.757  16.300   6.480  1.00 39.27           C
ATOM     50  O   GLY A  21      -0.309  15.895   6.908  1.00 38.03           O
ATOM     51  N   ALA A  22       1.005  17.584   6.240  1.00 38.86           N
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 52 | CA | ALA | A | 22 | -0.018 | 18.611 | 6.371 | 1.00 | 38.79 | C |
| ATOM | 53 | C | ALA | A | 22 | -0.618 | 18.613 | 7.758 | 1.00 | 38.64 | C |
| ATOM | 54 | O | ALA | A | 22 | -1.820 | 18.759 | 7.924 | 1.00 | 38.07 | O |
| ATOM | 55 | CB | ALA | A | 22 | -1.102 | 18.409 | 5.324 | 1.00 | 38.68 | C |
| ATOM | 56 | N | LEU | A | 23 | 0.231 | 18.451 | 8.760 | 1.00 | 39.07 | N |
| ATOM | 57 | CA | LEU | A | 23 | -0.233 | 18.473 | 10.135 | 1.00 | 39.72 | C |
| ATOM | 58 | C | LEU | A | 23 | -0.290 | 19.886 | 10.692 | 1.00 | 39.39 | C |
| ATOM | 59 | O | LEU | A | 23 | -0.464 | 20.075 | 11.880 | 1.00 | 39.41 | O |
| ATOM | 60 | CB | LEU | A | 23 | 0.642 | 17.574 | 11.003 | 1.00 | 40.11 | C |
| ATOM | 61 | CG | LEU | A | 23 | 0.528 | 16.118 | 10.558 | 1.00 | 41.82 | C |
| ATOM | 62 | CD1 | LEU | A | 23 | 1.414 | 15.185 | 11.384 | 1.00 | 43.18 | C |
| ATOM | 63 | CD2 | LEU | A | 23 | -0.916 | 15.673 | 10.633 | 1.00 | 43.43 | C |
| ATOM | 64 | N | GLY | A | 24 | -0.156 | 20.879 | 9.823 | 1.00 | 39.21 | N |
| ATOM | 65 | CA | GLY | A | 24 | -0.290 | 22.258 | 10.237 | 1.00 | 39.16 | C |
| ATOM | 66 | C | GLY | A | 24 | 0.964 | 22.862 | 10.820 | 1.00 | 39.21 | C |
| ATOM | 67 | O | GLY | A | 24 | 2.011 | 22.219 | 10.916 | 1.00 | 39.16 | O |
| ATOM | 68 | N | PRO | A | 25 | 0.854 | 24.118 | 11.223 | 1.00 | 39.08 | N |
| ATOM | 69 | CA | PRO | A | 25 | 1.997 | 24.830 | 11.775 | 1.00 | 38.84 | C |
| ATOM | 70 | C | PRO | A | 25 | 2.410 | 24.197 | 13.086 | 1.00 | 38.68 | C |
| ATOM | 71 | O | PRO | A | 25 | 1.572 | 23.842 | 13.914 | 1.00 | 38.08 | O |
| ATOM | 72 | CB | PRO | A | 25 | 1.477 | 26.259 | 12.001 | 1.00 | 38.76 | C |
| ATOM | 73 | CG | PRO | A | 25 | -0.004 | 26.197 | 11.895 | 1.00 | 39.12 | C |
| ATOM | 74 | CD | PRO | A | 25 | -0.375 | 24.930 | 11.210 | 1.00 | 39.17 | C |
| ATOM | 75 | N | ALA | A | 26 | 3.713 | 24.037 | 13.246 | 1.00 | 38.92 | N |
| ATOM | 76 | CA | ALA | A | 26 | 4.269 | 23.489 | 14.467 | 1.00 | 39.38 | C |
| ATOM | 77 | C | ALA | A | 26 | 3.924 | 24.381 | 15.676 | 1.00 | 38.73 | C |
| ATOM | 78 | O | ALA | A | 26 | 3.677 | 23.882 | 16.772 | 1.00 | 39.39 | O |
| ATOM | 79 | CB | ALA | A | 26 | 5.762 | 23.347 | 14.319 | 1.00 | 39.60 | C |
| ATOM | 80 | N | TRP | A | 27 | 3.871 | 25.687 | 15.468 | 1.00 | 37.43 | N |
| ATOM | 81 | CA | TRP | A | 27 | 3.516 | 26.602 | 16.543 | 1.00 | 36.82 | C |
| ATOM | 82 | C | TRP | A | 27 | 3.034 | 27.919 | 15.941 | 1.00 | 36.10 | C |
| ATOM | 83 | O | TRP | A | 27 | 3.013 | 28.074 | 14.731 | 1.00 | 35.54 | O |
| ATOM | 84 | CB | TRP | A | 27 | 4.746 | 26.835 | 17.424 | 1.00 | 36.91 | C |
| ATOM | 85 | CG | TRP | A | 27 | 5.949 | 27.019 | 16.596 | 1.00 | 36.01 | C |
| ATOM | 86 | CD1 | TRP | A | 27 | 6.770 | 26.041 | 16.089 | 1.00 | 36.29 | C |
| ATOM | 87 | CD2 | TRP | A | 27 | 6.450 | 28.249 | 16.107 | 1.00 | 34.41 | C |
| ATOM | 88 | NE1 | TRP | A | 27 | 7.761 | 26.610 | 15.324 | 1.00 | 36.06 | N |
| ATOM | 89 | CE2 | TRP | A | 27 | 7.592 | 27.966 | 15.332 | 1.00 | 34.97 | C |
| ATOM | 90 | CE3 | TRP | A | 27 | 6.066 | 29.568 | 16.263 | 1.00 | 34.24 | C |
| ATOM | 91 | CZ2 | TRP | A | 27 | 8.332 | 28.947 | 14.720 | 1.00 | 36.39 | C |
| ATOM | 92 | CZ3 | TRP | A | 27 | 6.808 | 30.539 | 15.664 | 1.00 | 36.24 | C |
| ATOM | 93 | CH2 | TRP | A | 27 | 7.927 | 30.225 | 14.890 | 1.00 | 36.25 | C |
| ATOM | 94 | N | ASP | A | 28 | 2.620 | 28.860 | 16.775 | 1.00 | 35.59 | N |
| ATOM | 95 | CA | ASP | A | 28 | 2.253 | 30.168 | 16.267 | 1.00 | 35.15 | C |
| ATOM | 96 | C | ASP | A | 28 | 2.816 | 31.224 | 17.160 | 1.00 | 33.93 | C |
| ATOM | 97 | O | ASP | A | 28 | 3.311 | 30.948 | 18.250 | 1.00 | 33.56 | O |
| ATOM | 98 | CB | ASP | A | 28 | 0.739 | 30.338 | 16.131 | 1.00 | 36.08 | C |
| ATOM | 99 | CG | ASP | A | 28 | 0.038 | 30.310 | 17.449 | 1.00 | 38.11 | C |
| ATOM | 100 | OD1 | ASP | A | 28 | -0.096 | 31.392 | 18.076 | 1.00 | 41.06 | O |
| ATOM | 101 | OD2 | ASP | A | 28 | -0.392 | 29.240 | 17.938 | 1.00 | 41.04 | O |
| ATOM | 102 | N | GLU | A | 29 | 2.737 | 32.448 | 16.665 | 1.00 | 32.84 | N |
| ATOM | 103 | CA | GLU | A | 29 | 3.288 | 33.615 | 17.330 | 1.00 | 31.31 | C |
| ATOM | 104 | C | GLU | A | 29 | 2.792 | 33.767 | 18.756 | 1.00 | 29.80 | C |
| ATOM | 105 | O | GLU | A | 29 | 3.547 | 34.124 | 19.639 | 1.00 | 29.03 | O |
| ATOM | 106 | CB | GLU | A | 29 | 2.938 | 34.841 | 16.537 | 1.00 | 31.81 | C |
| ATOM | 107 | N | SER | A | 30 | 1.524 | 33.478 | 18.989 | 1.00 | 28.55 | N |
| ATOM | 108 | CA | SER | A | 30 | 0.957 | 33.680 | 20.314 | 1.00 | 28.00 | C |
| ATOM | 109 | C | SER | A | 30 | 1.613 | 32.830 | 21.391 | 1.00 | 27.25 | C |
| ATOM | 110 | O | SER | A | 30 | 1.360 | 33.035 | 22.563 | 1.00 | 26.88 | O |
| ATOM | 111 | CB | SER | A | 30 | -0.546 | 33.404 | 20.302 | 1.00 | 27.71 | C |
| ATOM | 112 | OG | SER | A | 30 | -0.800 | 32.015 | 20.328 | 1.00 | 28.97 | O |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 113 | N | GLN | A | 31 | 2.434 | 31.864 | 20.994 | 1.00 | 26.92 | N |
| ATOM | 114 | CA | GLN | A | 31 | 3.089 | 30.988 | 21.950 | 1.00 | 26.85 | C |
| ATOM | 115 | C | GLN | A | 31 | 4.447 | 31.558 | 22.362 | 1.00 | 26.63 | C |
| ATOM | 116 | O | GLN | A | 31 | 5.115 | 30.995 | 23.220 | 1.00 | 25.89 | O |
| ATOM | 117 | CB | GLN | A | 31 | 3.270 | 29.576 | 21.375 | 1.00 | 26.90 | C |
| ATOM | 118 | CG | GLN | A | 31 | 1.975 | 28.816 | 21.097 | 1.00 | 27.50 | C |
| ATOM | 119 | CD | GLN | A | 31 | 2.227 | 27.446 | 20.480 | 1.00 | 27.30 | C |
| ATOM | 120 | OE1 | GLN | A | 31 | 2.332 | 27.330 | 19.262 | 1.00 | 28.39 | O |
| ATOM | 121 | NE2 | GLN | A | 31 | 2.354 | 26.419 | 21.319 | 1.00 | 23.43 | N |
| ATOM | 122 | N | LEU | A | 32 | 4.835 | 32.682 | 21.757 | 1.00 | 26.56 | N |
| ATOM | 123 | CA | LEU | A | 32 | 6.094 | 33.351 | 22.078 | 1.00 | 26.88 | C |
| ATOM | 124 | C | LEU | A | 32 | 5.854 | 34.500 | 23.047 | 1.00 | 26.64 | C |
| ATOM | 125 | O | LEU | A | 32 | 4.875 | 35.214 | 22.913 | 1.00 | 26.22 | O |
| ATOM | 126 | CB | LEU | A | 32 | 6.743 | 33.906 | 20.807 | 1.00 | 26.71 | C |
| ATOM | 127 | CG | LEU | A | 32 | 7.054 | 32.866 | 19.724 | 1.00 | 29.00 | C |
| ATOM | 128 | CD1 | LEU | A | 32 | 7.704 | 33.537 | 18.535 | 1.00 | 31.11 | C |
| ATOM | 129 | CD2 | LEU | A | 32 | 7.942 | 31.773 | 20.245 | 1.00 | 28.07 | C |
| ATOM | 130 | N | ARG | A | 33 | 6.737 | 34.671 | 24.026 | 1.00 | 26.49 | N |
| ATOM | 131 | CA | ARG | A | 33 | 6.622 | 35.799 | 24.957 | 1.00 | 26.48 | C |
| ATOM | 132 | C | ARG | A | 33 | 7.070 | 37.071 | 24.252 | 1.00 | 26.68 | C |
| ATOM | 133 | O | ARG | A | 33 | 7.810 | 37.025 | 23.280 | 1.00 | 26.97 | O |
| ATOM | 134 | CB | ARG | A | 33 | 7.454 | 35.554 | 26.224 | 1.00 | 26.44 | C |
| ATOM | 135 | CG | ARG | A | 33 | 7.071 | 34.261 | 26.976 | 1.00 | 25.53 | C |
| ATOM | 136 | CD | ARG | A | 33 | 7.869 | 34.029 | 28.245 | 1.00 | 25.76 | C |
| ATOM | 137 | NE | ARG | A | 33 | 7.329 | 32.926 | 29.021 | 1.00 | 25.87 | N |
| ATOM | 138 | CZ | ARG | A | 33 | 6.418 | 33.033 | 29.969 | 1.00 | 25.35 | C |
| ATOM | 139 | NH1 | ARG | A | 33 | 5.916 | 34.198 | 30.309 | 1.00 | 24.02 | N |
| ATOM | 140 | NH2 | ARG | A | 33 | 6.003 | 31.941 | 30.587 | 1.00 | 28.18 | N |
| ATOM | 141 | N | SER | A | 34 | 6.643 | 38.214 | 24.751 | 1.00 | 26.73 | N |
| ATOM | 142 | CA | SER | A | 34 | 6.939 | 39.469 | 24.090 | 1.00 | 27.21 | C |
| ATOM | 143 | C | SER | A | 34 | 8.021 | 40.251 | 24.840 | 1.00 | 26.40 | C |
| ATOM | 144 | O | SER | A | 34 | 7.957 | 40.391 | 26.046 | 1.00 | 25.65 | O |
| ATOM | 145 | CB | SER | A | 34 | 5.657 | 40.278 | 24.028 | 1.00 | 27.92 | C |
| ATOM | 146 | OG | SER | A | 34 | 5.402 | 40.780 | 25.323 | 1.00 | 31.78 | O |
| ATOM | 147 | N | TYR | A | 35 | 9.009 | 40.750 | 24.110 | 1.00 | 26.09 | N |
| ATOM | 148 | CA | TYR | A | 35 | 10.169 | 41.390 | 24.711 | 1.00 | 26.44 | C |
| ATOM | 149 | C | TYR | A | 35 | 10.412 | 42.731 | 24.046 | 1.00 | 27.00 | C |
| ATOM | 150 | O | TYR | A | 35 | 9.815 | 43.009 | 23.028 | 1.00 | 27.14 | O |
| ATOM | 151 | CB | TYR | A | 35 | 11.386 | 40.479 | 24.577 | 1.00 | 25.83 | C |
| ATOM | 152 | CG | TYR | A | 35 | 11.217 | 39.198 | 25.357 | 1.00 | 25.49 | C |
| ATOM | 153 | CD1 | TYR | A | 35 | 11.041 | 39.226 | 26.739 | 1.00 | 23.65 | C |
| ATOM | 154 | CD2 | TYR | A | 35 | 11.219 | 37.963 | 24.723 | 1.00 | 23.87 | C |
| ATOM | 155 | CE1 | TYR | A | 35 | 10.869 | 38.063 | 27.459 | 1.00 | 23.41 | C |
| ATOM | 156 | CE2 | TYR | A | 35 | 11.061 | 36.795 | 25.445 | 1.00 | 24.37 | C |
| ATOM | 157 | CZ | TYR | A | 35 | 10.881 | 36.847 | 26.809 | 1.00 | 22.92 | C |
| ATOM | 158 | OH | TYR | A | 35 | 10.698 | 35.686 | 27.522 | 1.00 | 23.94 | O |
| ATOM | 159 | N | SER | A | 36 | 11.326 | 43.531 | 24.596 | 1.00 | 27.45 | N |
| ATOM | 160 | CA | SER | A | 36 | 11.555 | 44.905 | 24.127 | 1.00 | 27.58 | C |
| ATOM | 161 | C | SER | A | 36 | 12.553 | 45.092 | 22.987 | 1.00 | 27.13 | C |
| ATOM | 162 | O | SER | A | 36 | 12.764 | 46.211 | 22.533 | 1.00 | 27.71 | O |
| ATOM | 163 | CB | SER | A | 36 | 12.109 | 45.724 | 25.286 | 1.00 | 27.62 | C |
| ATOM | 164 | OG | SER | A | 36 | 13.365 | 45.201 | 25.697 | 1.00 | 27.53 | O |
| ATOM | 165 | N | PHE | A | 37 | 13.181 | 44.025 | 22.543 | 1.00 | 25.62 | N |
| ATOM | 166 | CA | PHE | A | 37 | 14.263 | 44.169 | 21.590 | 1.00 | 24.95 | C |
| ATOM | 167 | C | PHE | A | 37 | 13.949 | 43.447 | 20.301 | 1.00 | 25.32 | C |
| ATOM | 168 | O | PHE | A | 37 | 13.191 | 42.512 | 20.274 | 1.00 | 25.29 | O |
| ATOM | 169 | CB | PHE | A | 37 | 15.537 | 43.571 | 22.185 | 1.00 | 23.88 | C |
| ATOM | 170 | CG | PHE | A | 37 | 15.340 | 42.162 | 22.731 | 1.00 | 22.69 | C |
| ATOM | 171 | CD1 | PHE | A | 37 | 15.353 | 41.077 | 21.890 | 1.00 | 20.43 | C |
| ATOM | 172 | CD2 | PHE | A | 37 | 15.104 | 41.949 | 24.076 | 1.00 | 23.12 | C |
| ATOM | 173 | CE1 | PHE | A | 37 | 15.160 | 39.778 | 22.386 | 1.00 | 22.83 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 174 | CE2 | PHE | A | 37 | 14.920 | 40.666 | 24.578 | 1.00 | 22.73 | C |
| ATOM | 175 | CZ | PHE | A | 37 | 14.944 | 39.585 | 23.737 | 1.00 | 22.04 | C |
| ATOM | 176 | N | PRO | A | 38 | 14.533 | 43.907 | 19.222 | 1.00 | 25.57 | N |
| ATOM | 177 | CA | PRO | A | 38 | 14.396 | 43.216 | 17.950 | 1.00 | 25.50 | C |
| ATOM | 178 | C | PRO | A | 38 | 15.321 | 42.002 | 17.861 | 1.00 | 25.35 | C |
| ATOM | 179 | O | PRO | A | 38 | 16.280 | 41.887 | 18.640 | 1.00 | 25.01 | O |
| ATOM | 180 | CB | PRO | A | 38 | 14.815 | 44.278 | 16.944 | 1.00 | 25.31 | C |
| ATOM | 181 | CG | PRO | A | 38 | 15.776 | 45.181 | 17.729 | 1.00 | 26.61 | C |
| ATOM | 182 | CD | PRO | A | 38 | 15.271 | 45.178 | 19.125 | 1.00 | 25.73 | C |
| ATOM | 183 | N | THR | A | 39 | 15.032 | 41.124 | 16.902 | 1.00 | 24.60 | N |
| ATOM | 184 | CA | THR | A | 39 | 15.876 | 39.979 | 16.607 | 1.00 | 24.58 | C |
| ATOM | 185 | C | THR | A | 39 | 15.881 | 39.686 | 15.112 | 1.00 | 25.39 | C |
| ATOM | 186 | O | THR | A | 39 | 15.004 | 40.121 | 14.383 | 1.00 | 24.72 | O |
| ATOM | 187 | CB | THR | A | 39 | 15.364 | 38.721 | 17.295 | 1.00 | 24.33 | C |
| ATOM | 188 | OG1 | THR | A | 39 | 14.023 | 38.453 | 16.860 | 1.00 | 21.36 | O |
| ATOM | 189 | CG2 | THR | A | 39 | 15.256 | 38.892 | 18.832 | 1.00 | 23.91 | C |
| ATOM | 190 | N | ARG | A | 40 | 16.875 | 38.912 | 14.692 | 1.00 | 26.09 | N |
| ATOM | 191 | CA | ARG | A | 40 | 17.000 | 38.399 | 13.337 | 1.00 | 26.92 | C |
| ATOM | 192 | C | ARG | A | 40 | 17.057 | 36.884 | 13.469 | 1.00 | 26.73 | C |
| ATOM | 193 | O | ARG | A | 40 | 17.407 | 36.366 | 14.517 | 1.00 | 26.53 | O |
| ATOM | 194 | CB | ARG | A | 40 | 18.291 | 38.888 | 12.696 | 1.00 | 27.12 | C |
| ATOM | 195 | CG | ARG | A | 40 | 18.289 | 40.360 | 12.400 | 1.00 | 32.37 | C |
| ATOM | 196 | CD | ARG | A | 40 | 16.925 | 40.858 | 11.994 | 1.00 | 36.79 | C |
| ATOM | 197 | NE | ARG | A | 40 | 16.783 | 41.137 | 10.583 | 1.00 | 41.20 | N |
| ATOM | 198 | CZ | ARG | A | 40 | 15.617 | 41.408 | 10.023 | 1.00 | 46.28 | C |
| ATOM | 199 | NH1 | ARG | A | 40 | 14.512 | 41.388 | 10.768 | 1.00 | 47.83 | N |
| ATOM | 200 | NH2 | ARG | A | 40 | 15.548 | 41.708 | 8.731 | 1.00 | 48.02 | N |
| ATOM | 201 | N | PRO | A | 41 | 16.728 | 36.163 | 12.413 | 1.00 | 26.96 | N |
| ATOM | 202 | CA | PRO | A | 41 | 16.709 | 34.706 | 12.510 | 1.00 | 27.17 | C |
| ATOM | 203 | C | PRO | A | 41 | 18.085 | 34.054 | 12.469 | 1.00 | 26.50 | C |
| ATOM | 204 | O | PRO | A | 41 | 19.002 | 34.538 | 11.830 | 1.00 | 26.34 | O |
| ATOM | 205 | CB | PRO | A | 41 | 15.867 | 34.277 | 11.298 | 1.00 | 27.12 | C |
| ATOM | 206 | CG | PRO | A | 41 | 16.027 | 35.434 | 10.296 | 1.00 | 27.66 | C |
| ATOM | 207 | CD | PRO | A | 41 | 16.337 | 36.661 | 11.077 | 1.00 | 26.70 | C |
| ATOM | 208 | N | ILE | A | 42 | 18.214 | 32.951 | 13.185 | 1.00 | 25.35 | N |
| ATOM | 209 | CA | ILE | A | 42 | 19.400 | 32.143 | 13.070 | 1.00 | 24.29 | C |
| ATOM | 210 | C | ILE | A | 42 | 19.161 | 31.290 | 11.832 | 1.00 | 23.98 | C |
| ATOM | 211 | O | ILE | A | 42 | 18.050 | 30.793 | 11.632 | 1.00 | 24.20 | O |
| ATOM | 212 | CB | ILE | A | 42 | 19.530 | 31.283 | 14.302 | 1.00 | 24.58 | C |
| ATOM | 213 | CG1 | ILE | A | 42 | 19.779 | 32.181 | 15.518 | 1.00 | 22.71 | C |
| ATOM | 214 | CG2 | ILE | A | 42 | 20.644 | 30.233 | 14.113 | 1.00 | 24.95 | C |
| ATOM | 215 | CD1 | ILE | A | 42 | 19.466 | 31.516 | 16.837 | 1.00 | 22.70 | C |
| ATOM | 216 | N | PRO | A | 43 | 20.168 | 31.122 | 10.989 | 1.00 | 23.44 | N |
| ATOM | 217 | CA | PRO | A | 43 | 20.016 | 30.276 | 9.807 | 1.00 | 23.74 | C |
| ATOM | 218 | C | PRO | A | 43 | 19.709 | 28.802 | 10.154 | 1.00 | 24.82 | C |
| ATOM | 219 | O | PRO | A | 43 | 20.281 | 28.292 | 11.130 | 1.00 | 24.03 | O |
| ATOM | 220 | CB | PRO | A | 43 | 21.372 | 30.397 | 9.107 | 1.00 | 24.23 | C |
| ATOM | 221 | CG | PRO | A | 43 | 22.071 | 31.602 | 9.740 | 1.00 | 23.91 | C |
| ATOM | 222 | CD | PRO | A | 43 | 21.504 | 31.737 | 11.092 | 1.00 | 23.12 | C |
| ATOM | 223 | N | ARG | A | 44 | 18.784 | 28.178 | 9.406 | 1.00 | 25.20 | N |
| ATOM | 224 | CA | ARG | A | 44 | 18.439 | 26.767 | 9.520 | 1.00 | 26.19 | C |
| ATOM | 225 | C | ARG | A | 44 | 18.977 | 26.125 | 8.269 | 1.00 | 25.69 | C |
| ATOM | 226 | O | ARG | A | 44 | 18.563 | 26.468 | 7.159 | 1.00 | 25.67 | O |
| ATOM | 227 | CB | ARG | A | 44 | 16.934 | 26.504 | 9.513 | 1.00 | 27.16 | C |
| ATOM | 228 | CG | ARG | A | 44 | 16.140 | 27.062 | 10.678 | 1.00 | 31.24 | C |
| ATOM | 229 | CD | ARG | A | 44 | 14.653 | 26.529 | 10.769 | 1.00 | 32.98 | C |
| ATOM | 230 | NE | ARG | A | 44 | 14.400 | 25.143 | 10.311 | 1.00 | 34.09 | N |
| ATOM | 231 | CZ | ARG | A | 44 | 14.258 | 24.070 | 11.128 | 1.00 | 33.28 | C |
| ATOM | 232 | NH1 | ARG | A | 44 | 14.384 | 24.177 | 12.453 | 1.00 | 29.63 | N |
| ATOM | 233 | NH2 | ARG | A | 44 | 13.995 | 22.873 | 10.617 | 1.00 | 34.28 | N |
| ATOM | 234 | N | LEU | A | 45 | 19.870 | 25.174 | 8.433 | 1.00 | 24.68 | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 235 | CA | LEU | A | 45 | 20.551 | 24.608 | 7.302 | 1.00 | 24.30 | C |
| ATOM | 236 | C | LEU | A | 45 | 20.768 | 23.134 | 7.471 | 1.00 | 24.39 | C |
| ATOM | 237 | O | LEU | A | 45 | 20.711 | 22.623 | 8.588 | 1.00 | 23.97 | O |
| ATOM | 238 | CB | LEU | A | 45 | 21.934 | 25.233 | 7.205 | 1.00 | 23.42 | C |
| ATOM | 239 | CG | LEU | A | 45 | 21.929 | 26.724 | 6.941 | 1.00 | 24.95 | C |
| ATOM | 240 | CD1 | LEU | A | 45 | 23.339 | 27.284 | 7.080 | 1.00 | 26.26 | C |
| ATOM | 241 | CD2 | LEU | A | 45 | 21.375 | 26.953 | 5.533 | 1.00 | 24.54 | C |
| ATOM | 242 | N | SER | A | 46 | 21.092 | 22.494 | 6.352 | 1.00 | 24.71 | N |
| ATOM | 243 | CA | SER | A | 46 | 21.498 | 21.119 | 6.345 | 1.00 | 25.24 | C |
| ATOM | 244 | C | SER | A | 46 | 22.930 | 21.043 | 6.804 | 1.00 | 25.58 | C |
| ATOM | 245 | O | SER | A | 46 | 23.741 | 21.908 | 6.522 | 1.00 | 24.65 | O |
| ATOM | 246 | CB | SER | A | 46 | 21.401 | 20.505 | 4.950 | 1.00 | 25.11 | C |
| ATOM | 247 | OG | SER | A | 46 | 21.863 | 19.150 | 4.965 | 1.00 | 24.50 | O |
| ATOM | 248 | N | GLN | A | 47 | 23.208 | 19.970 | 7.517 | 1.00 | 26.68 | N |
| ATOM | 249 | CA | GLN | A | 47 | 24.524 | 19.626 | 8.011 | 1.00 | 27.63 | C |
| ATOM | 250 | C | GLN | A | 47 | 25.510 | 19.442 | 6.853 | 1.00 | 28.01 | C |
| ATOM | 251 | O | GLN | A | 47 | 26.704 | 19.613 | 7.026 | 1.00 | 28.15 | O |
| ATOM | 252 | CB | GLN | A | 47 | 24.368 | 18.317 | 8.803 | 1.00 | 28.89 | C |
| ATOM | 253 | CG | GLN | A | 47 | 25.580 | 17.447 | 8.920 | 1.00 | 31.28 | C |
| ATOM | 254 | CD | GLN | A | 47 | 25.826 | 16.556 | 7.765 | 1.00 | 32.33 | C |
| ATOM | 255 | OE1 | GLN | A | 47 | 24.906 | 16.149 | 7.048 | 1.00 | 37.08 | O |
| ATOM | 256 | NE2 | GLN | A | 47 | 27.089 | 16.213 | 7.576 | 1.00 | 35.81 | N |
| ATOM | 257 | N | SER | A | 48 | 25.026 | 19.086 | 5.667 | 1.00 | 28.11 | N |
| ATOM | 258 | CA | SER | A | 48 | 25.930 | 18.925 | 4.524 | 1.00 | 28.72 | C |
| ATOM | 259 | C | SER | A | 48 | 26.222 | 20.262 | 3.828 | 1.00 | 29.21 | C |
| ATOM | 260 | O | SER | A | 48 | 27.068 | 20.339 | 2.936 | 1.00 | 29.21 | O |
| ATOM | 261 | CB | SER | A | 48 | 25.343 | 17.952 | 3.508 | 1.00 | 28.66 | C |
| ATOM | 262 | OG | SER | A | 48 | 24.111 | 18.440 | 2.993 | 1.00 | 29.43 | O |
| ATOM | 263 | N | ASP | A | 49 | 25.525 | 21.314 | 4.236 | 1.00 | 29.60 | N |
| ATOM | 264 | CA | ASP | A | 49 | 25.683 | 22.610 | 3.596 | 1.00 | 30.12 | C |
| ATOM | 265 | C | ASP | A | 49 | 26.949 | 23.307 | 4.087 | 1.00 | 30.43 | C |
| ATOM | 266 | O | ASP | A | 49 | 27.100 | 23.565 | 5.272 | 1.00 | 29.60 | O |
| ATOM | 267 | CB | ASP | A | 49 | 24.450 | 23.458 | 3.858 | 1.00 | 30.26 | C |
| ATOM | 268 | CG | ASP | A | 49 | 24.491 | 24.792 | 3.151 | 1.00 | 31.74 | C |
| ATOM | 269 | OD1 | ASP | A | 49 | 25.589 | 25.306 | 2.859 | 1.00 | 31.79 | O |
| ATOM | 270 | OD2 | ASP | A | 49 | 23.454 | 25.418 | 2.878 | 1.00 | 34.13 | O |
| ATOM | 271 | N | PRO | A | 50 | 27.829 | 23.668 | 3.155 | 1.00 | 31.31 | N |
| ATOM | 272 | CA | PRO | A | 50 | 29.123 | 24.273 | 3.499 | 1.00 | 31.63 | C |
| ATOM | 273 | C | PRO | A | 50 | 28.965 | 25.514 | 4.355 | 1.00 | 31.72 | C |
| ATOM | 274 | O | PRO | A | 50 | 29.849 | 25.807 | 5.164 | 1.00 | 31.85 | O |
| ATOM | 275 | CB | PRO | A | 50 | 29.726 | 24.643 | 2.124 | 1.00 | 31.53 | C |
| ATOM | 276 | CG | PRO | A | 50 | 29.036 | 23.738 | 1.168 | 1.00 | 32.13 | C |
| ATOM | 277 | CD | PRO | A | 50 | 27.624 | 23.620 | 1.697 | 1.00 | 31.55 | C |
| ATOM | 278 | N | ARG | A | 51 | 27.875 | 26.246 | 4.171 | 1.00 | 32.04 | N |
| ATOM | 279 | CA | ARG | A | 51 | 27.648 | 27.443 | 4.962 | 1.00 | 32.56 | C |
| ATOM | 280 | C | ARG | A | 51 | 27.478 | 27.078 | 6.439 | 1.00 | 32.09 | C |
| ATOM | 281 | O | ARG | A | 51 | 27.853 | 27.855 | 7.322 | 1.00 | 31.87 | O |
| ATOM | 282 | CB | ARG | A | 51 | 26.420 | 28.221 | 4.464 | 1.00 | 32.95 | C |
| ATOM | 283 | CG | ARG | A | 51 | 26.568 | 28.810 | 3.064 | 1.00 | 34.79 | C |
| ATOM | 284 | CD | ARG | A | 51 | 25.273 | 29.372 | 2.480 | 1.00 | 35.89 | C |
| ATOM | 285 | NE | ARG | A | 51 | 24.276 | 28.325 | 2.228 | 1.00 | 37.56 | N |
| ATOM | 286 | CZ | ARG | A | 51 | 22.982 | 28.564 | 2.061 | 1.00 | 39.54 | C |
| ATOM | 287 | NH1 | ARG | A | 51 | 22.531 | 29.814 | 2.124 | 1.00 | 40.85 | N |
| ATOM | 288 | NH2 | ARG | A | 51 | 22.135 | 27.573 | 1.823 | 1.00 | 38.55 | N |
| ATOM | 289 | N | ALA | A | 52 | 26.932 | 25.903 | 6.721 | 1.00 | 31.50 | N |
| ATOM | 290 | CA | ALA | A | 52 | 26.769 | 25.513 | 8.117 | 1.00 | 31.34 | C |
| ATOM | 291 | C | ALA | A | 52 | 28.135 | 25.310 | 8.744 | 1.00 | 31.24 | C |
| ATOM | 292 | O | ALA | A | 52 | 28.409 | 25.763 | 9.865 | 1.00 | 30.91 | O |
| ATOM | 293 | CB | ALA | A | 52 | 25.953 | 24.284 | 8.236 | 1.00 | 31.35 | C |
| ATOM | 294 | N | GLU | A | 53 | 29.005 | 24.652 | 8.005 | 1.00 | 30.92 | N |
| ATOM | 295 | CA | GLU | A | 53 | 30.332 | 24.404 | 8.501 | 1.00 | 31.92 | C |

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ATOM    296  C   GLU A  53      31.059  25.730   8.728  1.00 31.52           C
ATOM    297  O   GLU A  53      31.766  25.898   9.717  1.00 30.52           O
ATOM    298  CB  GLU A  53      31.119  23.554   7.525  1.00 32.10           C
ATOM    299  CG  GLU A  53      32.216  22.795   8.229  1.00 36.08           C
ATOM    300  CD  GLU A  53      31.776  21.411   8.717  1.00 39.44           C
ATOM    301  OE1 GLU A  53      30.629  21.234   9.167  1.00 40.34           O
ATOM    302  OE2 GLU A  53      32.606  20.487   8.652  1.00 43.45           O
ATOM    303  N   GLU A  54      30.870  26.665   7.808  1.00 31.32           N
ATOM    304  CA  GLU A  54      31.507  27.968   7.919  1.00 32.09           C
ATOM    305  C   GLU A  54      31.039  28.685   9.193  1.00 31.07           C
ATOM    306  O   GLU A  54      31.833  29.295   9.881  1.00 31.27           O
ATOM    307  CB  GLU A  54      31.218  28.812   6.681  1.00 32.42           C
ATOM    308  CG  GLU A  54      31.939  30.146   6.669  1.00 37.01           C
ATOM    309  CD  GLU A  54      31.662  30.966   5.410  1.00 40.45           C
ATOM    310  OE1 GLU A  54      30.843  30.528   4.558  1.00 41.94           O
ATOM    311  OE2 GLU A  54      32.268  32.051   5.285  1.00 43.43           O
ATOM    312  N   LEU A  55      29.761  28.567   9.534  1.00 29.85           N
ATOM    313  CA  LEU A  55      29.251  29.240  10.708  1.00 28.58           C
ATOM    314  C   LEU A  55      29.848  28.667  11.983  1.00 27.91           C
ATOM    315  O   LEU A  55      30.304  29.419  12.841  1.00 26.43           O
ATOM    316  CB  LEU A  55      27.734  29.179  10.733  1.00 28.61           C
ATOM    317  CG  LEU A  55      27.097  30.041   9.652  1.00 28.69           C
ATOM    318  CD1 LEU A  55      25.647  29.633   9.423  1.00 29.69           C
ATOM    319  CD2 LEU A  55      27.193  31.507  10.005  1.00 27.60           C
ATOM    320  N   ILE A  56      29.889  27.334  12.086  1.00 27.51           N
ATOM    321  CA  ILE A  56      30.432  26.679  13.278  1.00 27.49           C
ATOM    322  C   ILE A  56      31.910  27.014  13.457  1.00 28.32           C
ATOM    323  O   ILE A  56      32.359  27.353  14.549  1.00 28.51           O
ATOM    324  CB  ILE A  56      30.260  25.174  13.192  1.00 27.21           C
ATOM    325  CG1 ILE A  56      28.771  24.787  13.218  1.00 25.69           C
ATOM    326  CG2 ILE A  56      30.982  24.505  14.354  1.00 27.65           C
ATOM    327  CD1 ILE A  56      28.484  23.341  12.760  1.00 23.98           C
ATOM    328  N   GLU A  57      32.645  26.935  12.357  1.00 28.85           N
ATOM    329  CA  GLU A  57      34.068  27.230  12.308  1.00 29.98           C
ATOM    330  C   GLU A  57      34.319  28.623  12.837  1.00 30.12           C
ATOM    331  O   GLU A  57      35.306  28.869  13.524  1.00 31.00           O
ATOM    332  CB  GLU A  57      34.557  27.137  10.850  1.00 30.52           C
ATOM    333  CG  GLU A  57      36.003  27.518  10.610  1.00 33.37           C
ATOM    334  CD  GLU A  57      36.968  26.742  11.482  1.00 38.19           C
ATOM    335  OE1 GLU A  57      36.689  25.558  11.810  1.00 41.02           O
ATOM    336  OE2 GLU A  57      38.015  27.329  11.847  1.00 42.74           O
ATOM    337  N   ASN A  58      33.409  29.527  12.516  1.00 29.57           N
ATOM    338  CA  ASN A  58      33.516  30.911  12.929  1.00 29.62           C
ATOM    339  C   ASN A  58      32.852  31.222  14.230  1.00 27.88           C
ATOM    340  O   ASN A  58      32.690  32.364  14.566  1.00 26.74           O
ATOM    341  CB  ASN A  58      32.805  31.769  11.918  1.00 30.43           C
ATOM    342  CG  ASN A  58      33.719  32.439  11.040  1.00 33.87           C
ATOM    343  OD1 ASN A  58      34.040  31.918   9.965  1.00 36.67           O
ATOM    344  ND2 ASN A  58      34.189  33.629  11.467  1.00 38.66           N
ATOM    345  N   GLU A  59      32.396  30.205  14.922  1.00 27.73           N
ATOM    346  CA  GLU A  59      31.753  30.411  16.205  1.00 27.50           C
ATOM    347  C   GLU A  59      30.545  31.320  16.104  1.00 26.07           C
ATOM    348  O   GLU A  59      30.366  32.255  16.861  1.00 25.28           O
ATOM    349  CB  GLU A  59      32.795  30.867  17.224  1.00 28.12           C
ATOM    350  CG  GLU A  59      33.720  29.688  17.531  1.00 31.06           C
ATOM    351  CD  GLU A  59      34.739  29.965  18.604  1.00 35.24           C
ATOM    352  OE1 GLU A  59      35.826  30.432  18.239  1.00 39.24           O
ATOM    353  OE2 GLU A  59      34.469  29.698  19.795  1.00 37.54           O
ATOM    354  N   GLU A  60      29.691  30.982  15.155  1.00 25.70           N
ATOM    355  CA  GLU A  60      28.417  31.643  14.971  1.00 25.50           C
ATOM    356  C   GLU A  60      27.345  30.576  14.998  1.00 24.10           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 357 | O | GLU | A | 60 | 27.527 | 29.479 | 14.487 | 1.00 | 22.92 | O |
| ATOM | 358 | CB | GLU | A | 60 | 28.402 | 32.404 | 13.664 | 1.00 | 25.96 | C |
| ATOM | 359 | CG | GLU | A | 60 | 29.454 | 33.497 | 13.697 | 1.00 | 30.39 | C |
| ATOM | 360 | CD | GLU | A | 60 | 29.218 | 34.599 | 12.703 | 1.00 | 35.90 | C |
| ATOM | 361 | OE1 | GLU | A | 60 | 29.281 | 34.349 | 11.478 | 1.00 | 38.45 | O |
| ATOM | 362 | OE2 | GLU | A | 60 | 28.998 | 35.732 | 13.165 | 1.00 | 43.84 | O |
| ATOM | 363 | N | PRO | A | 61 | 26.203 | 30.933 | 15.546 | 1.00 | 22.92 | N |
| ATOM | 364 | CA | PRO | A | 61 | 25.112 | 29.983 | 15.735 | 1.00 | 22.31 | C |
| ATOM | 365 | C | PRO | A | 61 | 24.482 | 29.519 | 14.445 | 1.00 | 21.76 | C |
| ATOM | 366 | O | PRO | A | 61 | 24.394 | 30.252 | 13.474 | 1.00 | 21.59 | O |
| ATOM | 367 | CB | PRO | A | 61 | 24.079 | 30.775 | 16.525 | 1.00 | 22.55 | C |
| ATOM | 368 | CG | PRO | A | 61 | 24.450 | 32.218 | 16.380 | 1.00 | 21.42 | C |
| ATOM | 369 | CD | PRO | A | 61 | 25.863 | 32.295 | 15.967 | 1.00 | 22.38 | C |
| ATOM | 370 | N | VAL | A | 62 | 24.032 | 28.279 | 14.444 | 1.00 | 21.55 | N |
| ATOM | 371 | CA | VAL | A | 62 | 23.306 | 27.739 | 13.317 | 1.00 | 21.90 | C |
| ATOM | 372 | C | VAL | A | 62 | 22.415 | 26.622 | 13.817 | 1.00 | 22.38 | C |
| ATOM | 373 | O | VAL | A | 62 | 22.771 | 25.886 | 14.757 | 1.00 | 22.77 | O |
| ATOM | 374 | CB | VAL | A | 62 | 24.262 | 27.217 | 12.218 | 1.00 | 22.10 | C |
| ATOM | 375 | CG1 | VAL | A | 62 | 25.134 | 26.112 | 12.738 | 1.00 | 22.89 | C |
| ATOM | 376 | CG2 | VAL | A | 62 | 23.486 | 26.748 | 11.000 | 1.00 | 21.98 | C |
| ATOM | 377 | N | VAL | A | 63 | 21.234 | 26.517 | 13.226 | 1.00 | 22.90 | N |
| ATOM | 378 | CA | VAL | A | 63 | 20.373 | 25.398 | 13.499 | 1.00 | 23.20 | C |
| ATOM | 379 | C | VAL | A | 63 | 20.586 | 24.373 | 12.378 | 1.00 | 23.18 | C |
| ATOM | 380 | O | VAL | A | 63 | 20.395 | 24.682 | 11.208 | 1.00 | 23.38 | O |
| ATOM | 381 | CB | VAL | A | 63 | 18.880 | 25.768 | 13.561 | 1.00 | 23.27 | C |
| ATOM | 382 | CG1 | VAL | A | 63 | 18.046 | 24.483 | 13.754 | 1.00 | 24.19 | C |
| ATOM | 383 | CG2 | VAL | A | 63 | 18.620 | 26.695 | 14.692 | 1.00 | 22.51 | C |
| ATOM | 384 | N | LEU | A | 64 | 21.007 | 23.181 | 12.756 | 1.00 | 23.15 | N |
| ATOM | 385 | CA | LEU | A | 64 | 21.158 | 22.060 | 11.835 | 1.00 | 24.29 | C |
| ATOM | 386 | C | LEU | A | 64 | 19.904 | 21.203 | 11.906 | 1.00 | 23.48 | C |
| ATOM | 387 | O | LEU | A | 64 | 19.488 | 20.816 | 12.988 | 1.00 | 23.20 | O |
| ATOM | 388 | CB | LEU | A | 64 | 22.383 | 21.235 | 12.206 | 1.00 | 24.79 | C |
| ATOM | 389 | CG | LEU | A | 64 | 23.649 | 22.089 | 12.141 | 1.00 | 28.22 | C |
| ATOM | 390 | CD1 | LEU | A | 64 | 24.810 | 21.338 | 12.699 | 1.00 | 32.80 | C |
| ATOM | 391 | CD2 | LEU | A | 64 | 23.946 | 22.478 | 10.719 | 1.00 | 30.04 | C |
| ATOM | 392 | N | THR | A | 65 | 19.308 | 20.910 | 10.759 | 1.00 | 22.79 | N |
| ATOM | 393 | CA | THR | A | 65 | 18.019 | 20.218 | 10.740 | 1.00 | 23.27 | C |
| ATOM | 394 | C | THR | A | 65 | 18.088 | 18.730 | 10.534 | 1.00 | 23.05 | C |
| ATOM | 395 | O | THR | A | 65 | 17.102 | 18.050 | 10.765 | 1.00 | 22.85 | O |
| ATOM | 396 | CB | THR | A | 65 | 17.150 | 20.724 | 9.571 | 1.00 | 23.53 | C |
| ATOM | 397 | OG1 | THR | A | 65 | 17.855 | 20.496 | 8.352 | 1.00 | 22.75 | O |
| ATOM | 398 | CG2 | THR | A | 65 | 16.966 | 22.226 | 9.609 | 1.00 | 24.78 | C |
| ATOM | 399 | N | ASP | A | 66 | 19.231 | 18.227 | 10.093 | 1.00 | 23.33 | N |
| ATOM | 400 | CA | ASP | A | 66 | 19.330 | 16.828 | 9.731 | 1.00 | 23.76 | C |
| ATOM | 401 | C | ASP | A | 66 | 20.581 | 16.076 | 10.209 | 1.00 | 23.41 | C |
| ATOM | 402 | O | ASP | A | 66 | 21.117 | 15.265 | 9.457 | 1.00 | 23.64 | O |
| ATOM | 403 | CB | ASP | A | 66 | 19.245 | 16.732 | 8.199 | 1.00 | 23.97 | C |
| ATOM | 404 | CG | ASP | A | 66 | 20.326 | 17.517 | 7.514 | 1.00 | 24.64 | C |
| ATOM | 405 | OD1 | ASP | A | 66 | 21.175 | 18.099 | 8.223 | 1.00 | 23.06 | O |
| ATOM | 406 | OD2 | ASP | A | 66 | 20.417 | 17.612 | 6.268 | 1.00 | 26.54 | O |
| ATOM | 407 | N | THR | A | 67 | 21.050 | 16.336 | 11.428 | 1.00 | 22.72 | N |
| ATOM | 408 | CA | THR | A | 67 | 22.235 | 15.655 | 11.912 | 1.00 | 21.85 | C |
| ATOM | 409 | C | THR | A | 67 | 21.928 | 14.246 | 12.349 | 1.00 | 21.26 | C |
| ATOM | 410 | O | THR | A | 67 | 22.813 | 13.429 | 12.353 | 1.00 | 20.41 | O |
| ATOM | 411 | CB | THR | A | 67 | 22.836 | 16.345 | 13.138 | 1.00 | 21.92 | C |
| ATOM | 412 | OG1 | THR | A | 67 | 21.884 | 16.347 | 14.200 | 1.00 | 20.59 | O |
| ATOM | 413 | CG2 | THR | A | 67 | 23.161 | 17.822 | 12.873 | 1.00 | 23.29 | C |
| ATOM | 414 | N | ASN | A | 68 | 20.684 | 13.993 | 12.752 | 1.00 | 20.82 | N |
| ATOM | 415 | CA | ASN | A | 68 | 20.321 | 12.741 | 13.386 | 1.00 | 21.01 | C |
| ATOM | 416 | C | ASN | A | 68 | 21.146 | 12.525 | 14.652 | 1.00 | 20.47 | C |
| ATOM | 417 | O | ASN | A | 68 | 21.370 | 11.377 | 15.069 | 1.00 | 20.06 | O |

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ATOM    418  CB  ASN A  68      20.516  11.546  12.444  1.00 21.63           C
ATOM    419  CG  ASN A  68      19.476  11.493  11.340  1.00 22.28           C
ATOM    420  OD1 ASN A  68      18.276  11.429  11.601  1.00 23.83           O
ATOM    421  ND2 ASN A  68      19.936  11.492  10.108  1.00 22.82           N
ATOM    422  N   LEU A  69      21.613  13.617  15.248  1.00 19.86           N
ATOM    423  CA  LEU A  69      22.442  13.533  16.464  1.00 19.68           C
ATOM    424  C   LEU A  69      21.814  12.707  17.571  1.00 19.03           C
ATOM    425  O   LEU A  69      22.492  11.878  18.169  1.00 18.33           O
ATOM    426  CB  LEU A  69      22.770  14.907  17.009  1.00 19.89           C
ATOM    427  CG  LEU A  69      23.654  14.999  18.239  1.00 19.87           C
ATOM    428  CD1 LEU A  69      24.970  14.289  18.035  1.00 20.74           C
ATOM    429  CD2 LEU A  69      23.911  16.459  18.577  1.00 20.41           C
ATOM    430  N   VAL A  70      20.538  12.940  17.860  1.00 18.84           N
ATOM    431  CA  VAL A  70      19.843  12.177  18.894  1.00 18.85           C
ATOM    432  C   VAL A  70      18.634  11.447  18.339  1.00 19.17           C
ATOM    433  O   VAL A  70      17.604  11.325  19.000  1.00 18.71           O
ATOM    434  CB  VAL A  70      19.418  13.038  20.097  1.00 18.97           C
ATOM    435  CG1 VAL A  70      20.645  13.557  20.812  1.00 20.41           C
ATOM    436  CG2 VAL A  70      18.513  14.185  19.686  1.00 18.87           C
ATOM    437  N   TYR A  71      18.796  10.916  17.133  1.00 20.12           N
ATOM    438  CA  TYR A  71      17.711  10.224  16.454  1.00 20.64           C
ATOM    439  C   TYR A  71      17.003   9.218  17.377  1.00 20.76           C
ATOM    440  O   TYR A  71      15.804   9.275  17.507  1.00 20.54           O
ATOM    441  CB  TYR A  71      18.186   9.591  15.136  1.00 20.75           C
ATOM    442  CG  TYR A  71      17.243   8.517  14.628  1.00 23.02           C
ATOM    443  CD1 TYR A  71      16.012   8.837  14.046  1.00 24.62           C
ATOM    444  CD2 TYR A  71      17.572   7.182  14.754  1.00 22.94           C
ATOM    445  CE1 TYR A  71      15.132   7.800  13.595  1.00 23.64           C
ATOM    446  CE2 TYR A  71      16.730   6.174  14.312  1.00 23.48           C
ATOM    447  CZ  TYR A  71      15.524   6.478  13.730  1.00 24.03           C
ATOM    448  OH  TYR A  71      14.697   5.422  13.349  1.00 29.55           O
ATOM    449  N   PRO A  72      17.728   8.356  18.068  1.00 21.35           N
ATOM    450  CA  PRO A  72      17.080   7.363  18.945  1.00 21.89           C
ATOM    451  C   PRO A  72      16.296   7.955  20.106  1.00 22.22           C
ATOM    452  O   PRO A  72      15.432   7.269  20.628  1.00 21.25           O
ATOM    453  CB  PRO A  72      18.248   6.538  19.493  1.00 21.83           C
ATOM    454  CG  PRO A  72      19.420   6.849  18.606  1.00 22.53           C
ATOM    455  CD  PRO A  72      19.192   8.240  18.080  1.00 21.81           C
ATOM    456  N   ALA A  73      16.568   9.206  20.484  1.00 22.77           N
ATOM    457  CA  ALA A  73      15.859   9.836  21.605  1.00 23.23           C
ATOM    458  C   ALA A  73      14.542  10.487  21.178  1.00 23.64           C
ATOM    459  O   ALA A  73      13.764  10.966  22.014  1.00 23.47           O
ATOM    460  CB  ALA A  73      16.750  10.860  22.284  1.00 22.77           C
ATOM    461  N   LEU A  74      14.275  10.507  19.881  1.00 24.25           N
ATOM    462  CA  LEU A  74      13.057  11.148  19.405  1.00 24.86           C
ATOM    463  C   LEU A  74      11.792  10.466  19.920  1.00 25.46           C
ATOM    464  O   LEU A  74      10.729  11.070  19.967  1.00 25.11           O
ATOM    465  CB  LEU A  74      13.055  11.240  17.881  1.00 24.77           C
ATOM    466  CG  LEU A  74      14.160  12.161  17.338  1.00 26.74           C
ATOM    467  CD1 LEU A  74      13.915  12.478  15.867  1.00 28.86           C
ATOM    468  CD2 LEU A  74      14.288  13.447  18.135  1.00 26.86           C
ATOM    469  N   LYS A  75      11.908   9.204  20.306  1.00 26.12           N
ATOM    470  CA  LYS A  75      10.756   8.460  20.814  1.00 26.39           C
ATOM    471  C   LYS A  75      10.585   8.687  22.309  1.00 26.71           C
ATOM    472  O   LYS A  75       9.584   8.284  22.875  1.00 26.80           O
ATOM    473  CB  LYS A  75      10.918   6.963  20.534  1.00 26.36           C
ATOM    474  CG  LYS A  75      12.141   6.322  21.185  1.00 26.49           C
ATOM    475  CD  LYS A  75      12.254   4.813  20.838  1.00 27.59           C
ATOM    476  CE  LYS A  75      13.732   4.367  20.671  1.00 27.21           C
ATOM    477  NZ  LYS A  75      14.475   4.226  21.912  1.00 24.71           N
ATOM    478  N   TRP A  76      11.561   9.327  22.950  1.00 26.64           N
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 479 | CA | TRP | A | 76 | 11.484 | 9.557 | 24.383 | 1.00 | 26.78 | C |
| ATOM | 480 | C | TRP | A | 76 | 10.253 | 10.368 | 24.770 | 1.00 | 27.48 | C |
| ATOM | 481 | O | TRP | A | 76 | 9.889 | 11.317 | 24.095 | 1.00 | 27.93 | O |
| ATOM | 482 | CB | TRP | A | 76 | 12.717 | 10.311 | 24.888 | 1.00 | 26.57 | C |
| ATOM | 483 | CG | TRP | A | 76 | 13.963 | 9.500 | 24.895 | 1.00 | 25.80 | C |
| ATOM | 484 | CD1 | TRP | A | 76 | 14.101 | 8.219 | 24.486 | 1.00 | 24.26 | C |
| ATOM | 485 | CD2 | TRP | A | 76 | 15.255 | 9.917 | 25.347 | 1.00 | 22.71 | C |
| ATOM | 486 | NE1 | TRP | A | 76 | 15.399 | 7.804 | 24.647 | 1.00 | 23.20 | N |
| ATOM | 487 | CE2 | TRP | A | 76 | 16.128 | 8.829 | 25.178 | 1.00 | 22.53 | C |
| ATOM | 488 | CE3 | TRP | A | 76 | 15.767 | 11.107 | 25.867 | 1.00 | 21.96 | C |
| ATOM | 489 | CZ2 | TRP | A | 76 | 17.468 | 8.890 | 25.520 | 1.00 | 22.50 | C |
| ATOM | 490 | CZ3 | TRP | A | 76 | 17.090 | 11.172 | 26.202 | 1.00 | 20.53 | C |
| ATOM | 491 | CH2 | TRP | A | 76 | 17.931 | 10.076 | 26.029 | 1.00 | 22.36 | C |
| ATOM | 492 | N | ASP | A | 77 | 9.639 | 9.976 | 25.880 | 1.00 | 27.85 | N |
| ATOM | 493 | CA | ASP | A | 77 | 8.532 | 10.684 | 26.484 | 1.00 | 27.74 | C |
| ATOM | 494 | C | ASP | A | 77 | 8.560 | 10.277 | 27.957 | 1.00 | 27.45 | C |
| ATOM | 495 | O | ASP | A | 77 | 9.373 | 9.460 | 28.336 | 1.00 | 27.22 | O |
| ATOM | 496 | CB | ASP | A | 77 | 7.208 | 10.368 | 25.800 | 1.00 | 27.89 | C |
| ATOM | 497 | CG | ASP | A | 77 | 6.802 | 8.913 | 25.903 | 1.00 | 29.06 | C |
| ATOM | 498 | OD1 | ASP | A | 77 | 7.354 | 8.108 | 26.708 | 1.00 | 30.51 | O |
| ATOM | 499 | OD2 | ASP | A | 77 | 5.894 | 8.489 | 25.179 | 1.00 | 31.13 | O |
| ATOM | 500 | N | LEU | A | 78 | 7.710 | 10.847 | 28.796 | 1.00 | 27.47 | N |
| ATOM | 501 | CA | LEU | A | 78 | 7.819 | 10.578 | 30.229 | 1.00 | 27.63 | C |
| ATOM | 502 | C | LEU | A | 78 | 7.655 | 9.101 | 30.542 | 1.00 | 27.81 | C |
| ATOM | 503 | O | LEU | A | 78 | 8.386 | 8.548 | 31.367 | 1.00 | 27.16 | O |
| ATOM | 504 | CB | LEU | A | 78 | 6.818 | 11.409 | 31.011 | 1.00 | 27.59 | C |
| ATOM | 505 | CG | LEU | A | 78 | 7.007 | 12.916 | 30.880 | 1.00 | 28.68 | C |
| ATOM | 506 | CD1 | LEU | A | 78 | 5.906 | 13.677 | 31.612 | 1.00 | 28.95 | C |
| ATOM | 507 | CD2 | LEU | A | 78 | 8.369 | 13.328 | 31.412 | 1.00 | 29.32 | C |
| ATOM | 508 | N | GLU | A | 79 | 6.721 | 8.450 | 29.860 | 1.00 | 28.17 | N |
| ATOM | 509 | CA | GLU | A | 79 | 6.480 | 7.035 | 30.102 | 1.00 | 28.56 | C |
| ATOM | 510 | C | GLU | A | 79 | 7.715 | 6.185 | 29.781 | 1.00 | 28.22 | C |
| ATOM | 511 | O | GLU | A | 79 | 8.167 | 5.388 | 30.600 | 1.00 | 27.73 | O |
| ATOM | 512 | CB | GLU | A | 79 | 5.267 | 6.540 | 29.298 | 1.00 | 28.87 | C |
| ATOM | 513 | CG | GLU | A | 79 | 5.051 | 5.049 | 29.467 | 1.00 | 31.45 | C |
| ATOM | 514 | CD | GLU | A | 79 | 3.849 | 4.516 | 28.716 | 1.00 | 34.79 | C |
| ATOM | 515 | OE1 | GLU | A | 79 | 3.422 | 5.129 | 27.709 | 1.00 | 35.78 | O |
| ATOM | 516 | OE2 | GLU | A | 79 | 3.343 | 3.457 | 29.144 | 1.00 | 37.92 | O |
| ATOM | 517 | N | TYR | A | 80 | 8.260 | 6.346 | 28.582 | 1.00 | 28.27 | N |
| ATOM | 518 | CA | TYR | A | 80 | 9.452 | 5.597 | 28.200 | 1.00 | 28.00 | C |
| ATOM | 519 | C | TYR | A | 80 | 10.628 | 5.873 | 29.142 | 1.00 | 27.64 | C |
| ATOM | 520 | O | TYR | A | 80 | 11.330 | 4.958 | 29.563 | 1.00 | 27.16 | O |
| ATOM | 521 | CB | TYR | A | 80 | 9.838 | 5.964 | 26.787 | 1.00 | 28.13 | C |
| ATOM | 522 | CG | TYR | A | 80 | 11.054 | 5.250 | 26.246 | 1.00 | 27.95 | C |
| ATOM | 523 | CD1 | TYR | A | 80 | 10.952 | 3.991 | 25.644 | 1.00 | 27.39 | C |
| ATOM | 524 | CD2 | TYR | A | 80 | 12.300 | 5.846 | 26.306 | 1.00 | 25.55 | C |
| ATOM | 525 | CE1 | TYR | A | 80 | 12.089 | 3.352 | 25.128 | 1.00 | 26.82 | C |
| ATOM | 526 | CE2 | TYR | A | 80 | 13.417 | 5.224 | 25.808 | 1.00 | 25.50 | C |
| ATOM | 527 | CZ | TYR | A | 80 | 13.320 | 3.992 | 25.213 | 1.00 | 25.64 | C |
| ATOM | 528 | OH | TYR | A | 80 | 14.467 | 3.426 | 24.703 | 1.00 | 23.50 | O |
| ATOM | 529 | N | LEU | A | 81 | 10.839 | 7.135 | 29.482 | 1.00 | 27.51 | N |
| ATOM | 530 | CA | LEU | A | 81 | 11.952 | 7.477 | 30.371 | 1.00 | 27.75 | C |
| ATOM | 531 | C | LEU | A | 81 | 11.741 | 6.943 | 31.801 | 1.00 | 27.76 | C |
| ATOM | 532 | O | LEU | A | 81 | 12.682 | 6.459 | 32.437 | 1.00 | 27.35 | O |
| ATOM | 533 | CB | LEU | A | 81 | 12.194 | 8.990 | 30.399 | 1.00 | 27.35 | C |
| ATOM | 534 | CG | LEU | A | 81 | 12.659 | 9.656 | 29.096 | 1.00 | 28.06 | C |
| ATOM | 535 | CD1 | LEU | A | 81 | 12.664 | 11.170 | 29.269 | 1.00 | 28.55 | C |
| ATOM | 536 | CD2 | LEU | A | 81 | 14.036 | 9.192 | 28.655 | 1.00 | 27.65 | C |
| ATOM | 537 | N | GLN | A | 82 | 10.521 | 7.049 | 32.313 | 1.00 | 28.10 | N |
| ATOM | 538 | CA | GLN | A | 82 | 10.234 | 6.557 | 33.656 | 1.00 | 28.61 | C |
| ATOM | 539 | C | GLN | A | 82 | 10.525 | 5.066 | 33.689 | 1.00 | 28.32 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 540 | O | GLN | A | 82 | 11.070 | 4.550 | 34.643 | 1.00 | 28.25 | O |
| ATOM | 541 | CB | GLN | A | 82 | 8.774 | 6.805 | 34.032 | 1.00 | 29.04 | C |
| ATOM | 542 | CG | GLN | A | 82 | 8.325 | 6.063 | 35.293 | 1.00 | 30.18 | C |
| ATOM | 543 | CD | GLN | A | 82 | 7.184 | 6.754 | 36.042 | 1.00 | 32.25 | C |
| ATOM | 544 | OE1 | GLN | A | 82 | 6.642 | 7.758 | 35.594 | 1.00 | 34.51 | O |
| ATOM | 545 | NE2 | GLN | A | 82 | 6.822 | 6.204 | 37.189 | 1.00 | 36.79 | N |
| ATOM | 546 | N | GLU | A | 83 | 10.193 | 4.397 | 32.601 | 1.00 | 28.58 | N |
| ATOM | 547 | CA | GLU | A | 83 | 10.349 | 2.950 | 32.492 | 1.00 | 28.70 | C |
| ATOM | 548 | C | GLU | A | 83 | 11.801 | 2.515 | 32.314 | 1.00 | 28.14 | C |
| ATOM | 549 | O | GLU | A | 83 | 12.166 | 1.424 | 32.713 | 1.00 | 27.54 | O |
| ATOM | 550 | CB | GLU | A | 83 | 9.506 | 2.438 | 31.319 | 1.00 | 28.53 | C |
| ATOM | 551 | CG | GLU | A | 83 | 9.562 | 0.937 | 31.101 | 1.00 | 30.76 | C |
| ATOM | 552 | CD | GLU | A | 83 | 8.985 | 0.150 | 32.265 | 1.00 | 33.31 | C |
| ATOM | 553 | OE1 | GLU | A | 83 | 8.172 | 0.713 | 33.030 | 1.00 | 35.22 | O |
| ATOM | 554 | OE2 | GLU | A | 83 | 9.352 | -1.033 | 32.428 | 1.00 | 35.98 | O |
| ATOM | 555 | N | ASN | A | 84 | 12.644 | 3.374 | 31.753 | 1.00 | 27.44 | N |
| ATOM | 556 | CA | ASN | A | 84 | 13.985 | 2.938 | 31.400 | 1.00 | 27.09 | C |
| ATOM | 557 | C | ASN | A | 84 | 15.168 | 3.729 | 31.913 | 1.00 | 27.31 | C |
| ATOM | 558 | O | ASN | A | 84 | 16.291 | 3.276 | 31.759 | 1.00 | 27.17 | O |
| ATOM | 559 | CB | ASN | A | 84 | 14.099 | 2.917 | 29.879 | 1.00 | 27.17 | C |
| ATOM | 560 | CG | ASN | A | 84 | 13.226 | 1.890 | 29.254 | 1.00 | 26.24 | C |
| ATOM | 561 | OD1 | ASN | A | 84 | 13.361 | 0.696 | 29.532 | 1.00 | 27.49 | O |
| ATOM | 562 | ND2 | ASN | A | 84 | 12.312 | 2.333 | 28.413 | 1.00 | 23.37 | N |
| ATOM | 563 | N | ILE | A | 85 | 14.952 | 4.893 | 32.511 | 1.00 | 27.52 | N |
| ATOM | 564 | CA | ILE | A | 85 | 16.088 | 5.734 | 32.861 | 1.00 | 28.25 | C |
| ATOM | 565 | C | ILE | A | 85 | 16.788 | 5.390 | 34.185 | 1.00 | 28.03 | C |
| ATOM | 566 | O | ILE | A | 85 | 17.700 | 6.094 | 34.610 | 1.00 | 28.40 | O |
| ATOM | 567 | CB | ILE | A | 85 | 15.684 | 7.221 | 32.801 | 1.00 | 28.23 | C |
| ATOM | 568 | CG1 | ILE | A | 85 | 16.872 | 8.069 | 32.342 | 1.00 | 29.61 | C |
| ATOM | 569 | CG2 | ILE | A | 85 | 15.143 | 7.694 | 34.139 | 1.00 | 29.11 | C |
| ATOM | 570 | CD1 | ILE | A | 85 | 16.520 | 9.535 | 31.996 | 1.00 | 28.97 | C |
| ATOM | 571 | N | GLY | A | 86 | 16.368 | 4.317 | 34.833 | 1.00 | 28.14 | N |
| ATOM | 572 | CA | GLY | A | 86 | 17.014 | 3.874 | 36.061 | 1.00 | 28.15 | C |
| ATOM | 573 | C | GLY | A | 86 | 16.478 | 4.504 | 37.335 | 1.00 | 28.11 | C |
| ATOM | 574 | O | GLY | A | 86 | 15.494 | 5.251 | 37.308 | 1.00 | 27.93 | O |
| ATOM | 575 | N | ASN | A | 87 | 17.162 | 4.220 | 38.444 | 1.00 | 27.96 | N |
| ATOM | 576 | CA | ASN | A | 87 | 16.754 | 4.672 | 39.767 | 1.00 | 27.88 | C |
| ATOM | 577 | C | ASN | A | 87 | 17.736 | 5.677 | 40.373 | 1.00 | 27.82 | C |
| ATOM | 578 | O | ASN | A | 87 | 17.751 | 5.886 | 41.585 | 1.00 | 27.63 | O |
| ATOM | 579 | CB | ASN | A | 87 | 16.571 | 3.447 | 40.713 | 1.00 | 27.89 | C |
| ATOM | 580 | N | GLY | A | 88 | 18.559 | 6.301 | 39.538 | 1.00 | 28.21 | N |
| ATOM | 581 | CA | GLY | A | 88 | 19.478 | 7.336 | 40.006 | 1.00 | 28.18 | C |
| ATOM | 582 | C | GLY | A | 88 | 18.706 | 8.584 | 40.396 | 1.00 | 28.19 | C |
| ATOM | 583 | O | GLY | A | 88 | 17.520 | 8.676 | 40.097 | 1.00 | 28.62 | O |
| ATOM | 584 | N | ASP | A | 89 | 19.357 | 9.530 | 41.068 | 1.00 | 27.99 | N |
| ATOM | 585 | CA | ASP | A | 89 | 18.707 | 10.781 | 41.468 | 1.00 | 28.09 | C |
| ATOM | 586 | C | ASP | A | 89 | 18.655 | 11.806 | 40.335 | 1.00 | 28.00 | C |
| ATOM | 587 | O | ASP | A | 89 | 19.557 | 11.866 | 39.507 | 1.00 | 28.07 | O |
| ATOM | 588 | CB | ASP | A | 89 | 19.467 | 11.433 | 42.613 | 1.00 | 28.24 | C |
| ATOM | 589 | CG | ASP | A | 89 | 19.249 | 10.747 | 43.935 | 1.00 | 28.53 | C |
| ATOM | 590 | OD1 | ASP | A | 89 | 18.398 | 9.843 | 44.024 | 1.00 | 30.26 | O |
| ATOM | 591 | OD2 | ASP | A | 89 | 19.884 | 11.070 | 44.955 | 1.00 | 29.31 | O |
| ATOM | 592 | N | PHE | A | 90 | 17.620 | 12.637 | 40.330 | 1.00 | 27.56 | N |
| ATOM | 593 | CA | PHE | A | 90 | 17.510 | 13.687 | 39.332 | 1.00 | 27.37 | C |
| ATOM | 594 | C | PHE | A | 90 | 17.291 | 15.037 | 39.993 | 1.00 | 27.78 | C |
| ATOM | 595 | O | PHE | A | 90 | 16.453 | 15.171 | 40.884 | 1.00 | 27.69 | O |
| ATOM | 596 | CB | PHE | A | 90 | 16.378 | 13.388 | 38.351 | 1.00 | 27.05 | C |
| ATOM | 597 | CG | PHE | A | 90 | 16.678 | 12.262 | 37.408 | 1.00 | 25.85 | C |
| ATOM | 598 | CD1 | PHE | A | 90 | 16.525 | 10.943 | 37.806 | 1.00 | 25.70 | C |
| ATOM | 599 | CD2 | PHE | A | 90 | 17.119 | 12.521 | 36.121 | 1.00 | 26.20 | C |
| ATOM | 600 | CE1 | PHE | A | 90 | 16.797 | 9.908 | 36.943 | 1.00 | 24.06 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 601 | CE2 | PHE | A | 90 | 17.395 | 11.489 | 35.248 | 1.00 | 25.49 | C |
| ATOM | 602 | CZ | PHE | A | 90 | 17.235 | 10.176 | 35.666 | 1.00 | 25.33 | C |
| ATOM | 603 | N | SER | A | 91 | 18.062 | 16.033 | 39.560 | 1.00 | 27.85 | N |
| ATOM | 604 | CA | SER | A | 91 | 17.902 | 17.384 | 40.075 | 1.00 | 28.17 | C |
| ATOM | 605 | C | SER | A | 91 | 16.695 | 18.023 | 39.419 | 1.00 | 28.48 | C |
| ATOM | 606 | O | SER | A | 91 | 16.589 | 18.085 | 38.192 | 1.00 | 28.35 | O |
| ATOM | 607 | CB | SER | A | 91 | 19.149 | 18.236 | 39.838 | 1.00 | 27.86 | C |
| ATOM | 608 | OG | SER | A | 91 | 20.260 | 17.652 | 40.485 | 1.00 | 27.15 | O |
| ATOM | 609 | N | VAL | A | 92 | 15.784 | 18.482 | 40.261 | 1.00 | 29.05 | N |
| ATOM | 610 | CA | VAL | A | 92 | 14.585 | 19.141 | 39.812 | 1.00 | 29.67 | C |
| ATOM | 611 | C | VAL | A | 92 | 14.437 | 20.465 | 40.529 | 1.00 | 30.31 | C |
| ATOM | 612 | O | VAL | A | 92 | 14.442 | 20.537 | 41.763 | 1.00 | 30.37 | O |
| ATOM | 613 | CB | VAL | A | 92 | 13.352 | 18.313 | 40.106 | 1.00 | 29.81 | C |
| ATOM | 614 | CG1 | VAL | A | 92 | 12.106 | 19.026 | 39.582 | 1.00 | 29.93 | C |
| ATOM | 615 | CG2 | VAL | A | 92 | 13.490 | 16.930 | 39.507 | 1.00 | 29.60 | C |
| ATOM | 616 | N | TYR | A | 93 | 14.329 | 21.516 | 39.732 | 1.00 | 31.00 | N |
| ATOM | 617 | CA | TYR | A | 93 | 14.135 | 22.845 | 40.241 | 1.00 | 31.29 | C |
| ATOM | 618 | C | TYR | A | 93 | 12.662 | 23.113 | 40.298 | 1.00 | 31.54 | C |
| ATOM | 619 | O | TYR | A | 93 | 11.892 | 22.701 | 39.423 | 1.00 | 31.35 | O |
| ATOM | 620 | CB | TYR | A | 93 | 14.829 | 23.853 | 39.345 | 1.00 | 31.87 | C |
| ATOM | 621 | CG | TYR | A | 93 | 16.310 | 23.711 | 39.436 | 1.00 | 33.05 | C |
| ATOM | 622 | CD1 | TYR | A | 93 | 17.012 | 24.283 | 40.482 | 1.00 | 34.67 | C |
| ATOM | 623 | CD2 | TYR | A | 93 | 16.998 | 22.954 | 38.525 | 1.00 | 34.24 | C |
| ATOM | 624 | CE1 | TYR | A | 93 | 18.357 | 24.125 | 40.593 | 1.00 | 35.09 | C |
| ATOM | 625 | CE2 | TYR | A | 93 | 18.338 | 22.789 | 38.634 | 1.00 | 36.36 | C |
| ATOM | 626 | CZ | TYR | A | 93 | 19.011 | 23.379 | 39.670 | 1.00 | 36.33 | C |
| ATOM | 627 | OH | TYR | A | 93 | 20.357 | 23.204 | 39.772 | 1.00 | 40.81 | O |
| ATOM | 628 | N | SER | A | 94 | 12.286 | 23.813 | 41.351 | 1.00 | 32.03 | N |
| ATOM | 629 | CA | SER | A | 94 | 10.919 | 24.182 | 41.599 | 1.00 | 32.31 | C |
| ATOM | 630 | C | SER | A | 94 | 10.884 | 25.692 | 41.704 | 1.00 | 32.42 | C |
| ATOM | 631 | O | SER | A | 94 | 11.743 | 26.286 | 42.350 | 1.00 | 32.48 | O |
| ATOM | 632 | CB | SER | A | 94 | 10.464 | 23.566 | 42.914 | 1.00 | 32.38 | C |
| ATOM | 633 | OG | SER | A | 94 | 9.062 | 23.691 | 43.052 | 1.00 | 33.53 | O |
| ATOM | 634 | N | ALA | A | 95 | 9.902 | 26.314 | 41.070 | 1.00 | 32.58 | N |
| ATOM | 635 | CA | ALA | A | 95 | 9.766 | 27.757 | 41.135 | 1.00 | 32.90 | C |
| ATOM | 636 | C | ALA | A | 95 | 8.312 | 28.172 | 41.076 | 1.00 | 33.48 | C |
| ATOM | 637 | O | ALA | A | 95 | 7.446 | 27.429 | 40.620 | 1.00 | 33.62 | O |
| ATOM | 638 | CB | ALA | A | 95 | 10.528 | 28.413 | 39.996 | 1.00 | 32.80 | C |
| ATOM | 639 | N | SER | A | 96 | 8.053 | 29.382 | 41.539 | 1.00 | 34.08 | N |
| ATOM | 640 | CA | SER | A | 96 | 6.721 | 29.932 | 41.482 | 1.00 | 34.75 | C |
| ATOM | 641 | C | SER | A | 96 | 6.616 | 30.974 | 40.382 | 1.00 | 34.55 | C |
| ATOM | 642 | O | SER | A | 96 | 5.603 | 31.659 | 40.275 | 1.00 | 35.29 | O |
| ATOM | 643 | CB | SER | A | 96 | 6.363 | 30.592 | 42.801 | 1.00 | 35.05 | C |
| ATOM | 644 | OG | SER | A | 96 | 5.165 | 31.311 | 42.627 | 1.00 | 36.18 | O |
| ATOM | 645 | N | THR | A | 97 | 7.673 | 31.107 | 39.593 | 1.00 | 33.88 | N |
| ATOM | 646 | CA | THR | A | 97 | 7.716 | 32.046 | 38.477 | 1.00 | 33.41 | C |
| ATOM | 647 | C | THR | A | 97 | 8.084 | 31.238 | 37.265 | 1.00 | 32.32 | C |
| ATOM | 648 | O | THR | A | 97 | 8.590 | 30.143 | 37.411 | 1.00 | 32.10 | O |
| ATOM | 649 | CB | THR | A | 97 | 8.797 | 33.144 | 38.695 | 1.00 | 33.64 | C |
| ATOM | 650 | OG1 | THR | A | 97 | 9.067 | 33.810 | 37.460 | 1.00 | 33.76 | O |
| ATOM | 651 | CG2 | THR | A | 97 | 10.190 | 32.559 | 39.058 | 1.00 | 34.25 | C |
| ATOM | 652 | N | HIS | A | 98 | 7.840 | 31.762 | 36.073 | 1.00 | 31.47 | N |
| ATOM | 653 | CA | HIS | A | 98 | 8.278 | 31.071 | 34.863 | 1.00 | 30.97 | C |
| ATOM | 654 | C | HIS | A | 98 | 9.804 | 31.134 | 34.707 | 1.00 | 30.53 | C |
| ATOM | 655 | O | HIS | A | 98 | 10.378 | 30.379 | 33.940 | 1.00 | 29.14 | O |
| ATOM | 656 | CB | HIS | A | 98 | 7.613 | 31.666 | 33.621 | 1.00 | 31.14 | C |
| ATOM | 657 | CG | HIS | A | 98 | 7.878 | 33.125 | 33.415 | 1.00 | 30.86 | C |
| ATOM | 658 | ND1 | HIS | A | 98 | 7.121 | 34.112 | 34.011 | 1.00 | 31.51 | N |
| ATOM | 659 | CD2 | HIS | A | 98 | 8.795 | 33.767 | 32.651 | 1.00 | 31.48 | C |
| ATOM | 660 | CE1 | HIS | A | 98 | 7.566 | 35.298 | 33.634 | 1.00 | 31.14 | C |
| ATOM | 661 | NE2 | HIS | A | 98 | 8.581 | 35.118 | 32.805 | 1.00 | 30.50 | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 662 | N | LYS | A | 99 | 10.459 | 32.025 | 35.449 | 1.00 | 30.36 | N |
| ATOM | 663 | CA | LYS | A | 99 | 11.895 | 32.198 | 35.298 | 1.00 | 31.07 | C |
| ATOM | 664 | C | LYS | A | 99 | 12.761 | 31.288 | 36.166 | 1.00 | 31.00 | C |
| ATOM | 665 | O | LYS | A | 99 | 12.693 | 31.337 | 37.396 | 1.00 | 31.91 | O |
| ATOM | 666 | CB | LYS | A | 99 | 12.265 | 33.643 | 35.544 | 1.00 | 31.15 | C |
| ATOM | 667 | CG | LYS | A | 99 | 11.887 | 34.551 | 34.391 | 1.00 | 33.39 | C |
| ATOM | 668 | CD | LYS | A | 99 | 12.486 | 35.945 | 34.556 | 1.00 | 36.16 | C |
| ATOM | 669 | CE | LYS | A | 99 | 11.763 | 36.771 | 35.607 | 1.00 | 37.52 | C |
| ATOM | 670 | NZ | LYS | A | 99 | 10.620 | 37.507 | 35.006 | 1.00 | 38.84 | N |
| ATOM | 671 | N | PHE | A | 100 | 13.572 | 30.453 | 35.518 | 1.00 | 30.20 | N |
| ATOM | 672 | CA | PHE | A | 100 | 14.517 | 29.606 | 36.232 | 1.00 | 30.03 | C |
| ATOM | 673 | C | PHE | A | 100 | 15.952 | 30.123 | 36.138 | 1.00 | 29.72 | C |
| ATOM | 674 | O | PHE | A | 100 | 16.826 | 29.544 | 35.481 | 1.00 | 29.39 | O |
| ATOM | 675 | CB | PHE | A | 100 | 14.441 | 28.168 | 35.744 | 1.00 | 29.93 | C |
| ATOM | 676 | CG | PHE | A | 100 | 13.223 | 27.452 | 36.206 | 1.00 | 29.72 | C |
| ATOM | 677 | CD1 | PHE | A | 100 | 12.014 | 27.637 | 35.566 | 1.00 | 28.98 | C |
| ATOM | 678 | CD2 | PHE | A | 100 | 13.283 | 26.596 | 37.289 | 1.00 | 30.77 | C |
| ATOM | 679 | CE1 | PHE | A | 100 | 10.896 | 26.969 | 35.983 | 1.00 | 30.22 | C |
| ATOM | 680 | CE2 | PHE | A | 100 | 12.158 | 25.919 | 37.719 | 1.00 | 30.51 | C |
| ATOM | 681 | CZ | PHE | A | 100 | 10.967 | 26.105 | 37.069 | 1.00 | 30.63 | C |
| ATOM | 682 | N | LEU | A | 101 | 16.178 | 31.235 | 36.809 | 1.00 | 29.87 | N |
| ATOM | 683 | CA | LEU | A | 101 | 17.495 | 31.812 | 36.919 | 1.00 | 29.57 | C |
| ATOM | 684 | C | LEU | A | 101 | 18.451 | 30.814 | 37.555 | 1.00 | 29.61 | C |
| ATOM | 685 | O | LEU | A | 101 | 18.249 | 30.380 | 38.679 | 1.00 | 28.35 | O |
| ATOM | 686 | CB | LEU | A | 101 | 17.412 | 33.057 | 37.787 | 1.00 | 29.68 | C |
| ATOM | 687 | CG | LEU | A | 101 | 18.707 | 33.845 | 37.954 | 1.00 | 29.68 | C |
| ATOM | 688 | CD1 | LEU | A | 101 | 19.184 | 34.337 | 36.620 | 1.00 | 28.70 | C |
| ATOM | 689 | CD2 | LEU | A | 101 | 18.474 | 35.014 | 38.909 | 1.00 | 31.41 | C |
| ATOM | 690 | N | TYR | A | 102 | 19.490 | 30.440 | 36.816 | 1.00 | 30.36 | N |
| ATOM | 691 | CA | TYR | A | 102 | 20.516 | 29.535 | 37.338 | 1.00 | 30.64 | C |
| ATOM | 692 | C | TYR | A | 102 | 21.332 | 30.228 | 38.440 | 1.00 | 30.93 | C |
| ATOM | 693 | O | TYR | A | 102 | 21.623 | 31.425 | 38.339 | 1.00 | 30.67 | O |
| ATOM | 694 | CB | TYR | A | 102 | 21.480 | 29.101 | 36.224 | 1.00 | 30.45 | C |
| ATOM | 695 | CG | TYR | A | 102 | 22.609 | 28.271 | 36.774 | 1.00 | 31.25 | C |
| ATOM | 696 | CD1 | TYR | A | 102 | 22.430 | 26.916 | 37.062 | 1.00 | 31.33 | C |
| ATOM | 697 | CD2 | TYR | A | 102 | 23.842 | 28.844 | 37.054 | 1.00 | 31.29 | C |
| ATOM | 698 | CE1 | TYR | A | 102 | 23.456 | 26.163 | 37.612 | 1.00 | 32.81 | C |
| ATOM | 699 | CE2 | TYR | A | 102 | 24.869 | 28.098 | 37.601 | 1.00 | 32.24 | C |
| ATOM | 700 | CZ | TYR | A | 102 | 24.676 | 26.764 | 37.876 | 1.00 | 34.18 | C |
| ATOM | 701 | OH | TYR | A | 102 | 25.720 | 26.030 | 38.418 | 1.00 | 39.06 | O |
| ATOM | 702 | N | TYR | A | 103 | 21.684 | 29.478 | 39.488 | 1.00 | 31.28 | N |
| ATOM | 703 | CA | TYR | A | 103 | 22.569 | 29.983 | 40.539 | 1.00 | 31.56 | C |
| ATOM | 704 | C | TYR | A | 103 | 23.524 | 28.911 | 41.058 | 1.00 | 31.11 | C |
| ATOM | 705 | O | TYR | A | 103 | 23.190 | 27.732 | 41.165 | 1.00 | 30.75 | O |
| ATOM | 706 | CB | TYR | A | 103 | 21.796 | 30.599 | 41.706 | 1.00 | 31.98 | C |
| ATOM | 707 | CG | TYR | A | 103 | 20.846 | 29.663 | 42.385 | 1.00 | 33.92 | C |
| ATOM | 708 | CD1 | TYR | A | 103 | 19.577 | 29.445 | 41.868 | 1.00 | 36.08 | C |
| ATOM | 709 | CD2 | TYR | A | 103 | 21.203 | 29.010 | 43.553 | 1.00 | 36.91 | C |
| ATOM | 710 | CE1 | TYR | A | 103 | 18.696 | 28.587 | 42.483 | 1.00 | 37.42 | C |
| ATOM | 711 | CE2 | TYR | A | 103 | 20.325 | 28.153 | 44.189 | 1.00 | 37.63 | C |
| ATOM | 712 | CZ | TYR | A | 103 | 19.070 | 27.947 | 43.647 | 1.00 | 38.74 | C |
| ATOM | 713 | OH | TYR | A | 103 | 18.183 | 27.099 | 44.264 | 1.00 | 40.90 | O |
| ATOM | 714 | N | ASP | A | 104 | 24.725 | 29.345 | 41.391 | 1.00 | 30.34 | N |
| ATOM | 715 | CA | ASP | A | 104 | 25.752 | 28.444 | 41.873 | 1.00 | 30.04 | C |
| ATOM | 716 | C | ASP | A | 104 | 25.735 | 28.408 | 43.394 | 1.00 | 29.73 | C |
| ATOM | 717 | O | ASP | A | 104 | 26.079 | 29.388 | 44.062 | 1.00 | 28.53 | O |
| ATOM | 718 | CB | ASP | A | 104 | 27.089 | 28.931 | 41.350 | 1.00 | 30.07 | C |
| ATOM | 719 | CG | ASP | A | 104 | 28.233 | 28.037 | 41.731 | 1.00 | 30.02 | C |
| ATOM | 720 | OD1 | ASP | A | 104 | 28.069 | 27.137 | 42.605 | 1.00 | 28.92 | O |
| ATOM | 721 | OD2 | ASP | A | 104 | 29.339 | 28.183 | 41.168 | 1.00 | 29.24 | O |
| ATOM | 722 | N | GLU | A | 105 | 25.327 | 27.263 | 43.931 | 1.00 | 29.74 | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 723 | CA | GLU | A | 105 | 25.169 | 27.095 | 45.371 | 1.00 | 29.91 | C |
| ATOM | 724 | C | GLU | A | 105 | 26.461 | 27.343 | 46.155 | 1.00 | 29.29 | C |
| ATOM | 725 | O | GLU | A | 105 | 26.412 | 27.872 | 47.263 | 1.00 | 28.37 | O |
| ATOM | 726 | CB | GLU | A | 105 | 24.601 | 25.699 | 45.672 | 1.00 | 30.40 | C |
| ATOM | 727 | CG | GLU | A | 105 | 23.097 | 25.621 | 45.410 | 1.00 | 32.58 | C |
| ATOM | 728 | CD | GLU | A | 105 | 22.546 | 24.210 | 45.287 | 1.00 | 34.72 | C |
| ATOM | 729 | OE1 | GLU | A | 105 | 22.945 | 23.320 | 46.072 | 1.00 | 35.38 | O |
| ATOM | 730 | OE2 | GLU | A | 105 | 21.683 | 24.001 | 44.402 | 1.00 | 35.93 | O |
| ATOM | 731 | N | LYS | A | 106 | 27.607 | 27.000 | 45.565 | 1.00 | 29.02 | N |
| ATOM | 732 | CA | LYS | A | 106 | 28.897 | 27.156 | 46.243 | 1.00 | 29.26 | C |
| ATOM | 733 | C | LYS | A | 106 | 29.245 | 28.608 | 46.493 | 1.00 | 29.31 | C |
| ATOM | 734 | O | LYS | A | 106 | 30.051 | 28.903 | 47.363 | 1.00 | 28.83 | O |
| ATOM | 735 | CB | LYS | A | 106 | 30.036 | 26.530 | 45.433 | 1.00 | 29.60 | C |
| ATOM | 736 | CG | LYS | A | 106 | 29.864 | 25.036 | 45.094 | 1.00 | 30.18 | C |
| ATOM | 737 | N | LYS | A | 107 | 28.646 | 29.516 | 45.724 | 1.00 | 29.27 | N |
| ATOM | 738 | CA | LYS | A | 107 | 28.925 | 30.933 | 45.876 | 1.00 | 29.61 | C |
| ATOM | 739 | C | LYS | A | 107 | 27.933 | 31.605 | 46.820 | 1.00 | 30.29 | C |
| ATOM | 740 | O | LYS | A | 107 | 28.062 | 32.785 | 47.100 | 1.00 | 30.16 | O |
| ATOM | 741 | CB | LYS | A | 107 | 28.924 | 31.636 | 44.504 | 1.00 | 29.35 | C |
| ATOM | 742 | CG | LYS | A | 107 | 30.222 | 31.411 | 43.697 | 1.00 | 28.97 | C |
| ATOM | 743 | CD | LYS | A | 107 | 30.142 | 31.864 | 42.230 | 1.00 | 26.18 | C |
| ATOM | 744 | CE | LYS | A | 107 | 31.459 | 31.534 | 41.498 | 1.00 | 26.51 | C |
| ATOM | 745 | NZ | LYS | A | 107 | 31.578 | 32.052 | 40.083 | 1.00 | 24.21 | N |
| ATOM | 746 | N | MET | A | 108 | 26.950 | 30.869 | 47.320 | 1.00 | 31.39 | N |
| ATOM | 747 | CA | MET | A | 108 | 25.939 | 31.482 | 48.186 | 1.00 | 32.74 | C |
| ATOM | 748 | C | MET | A | 108 | 26.468 | 32.050 | 49.514 | 1.00 | 33.50 | C |
| ATOM | 749 | O | MET | A | 108 | 25.987 | 33.082 | 49.988 | 1.00 | 33.27 | O |
| ATOM | 750 | CB | MET | A | 108 | 24.787 | 30.509 | 48.417 | 1.00 | 33.11 | C |
| ATOM | 751 | CG | MET | A | 108 | 23.976 | 30.300 | 47.127 | 1.00 | 34.43 | C |
| ATOM | 752 | SD | MET | A | 108 | 22.458 | 29.330 | 47.263 | 1.00 | 37.47 | S |
| ATOM | 753 | CE | MET | A | 108 | 21.487 | 30.326 | 48.417 | 1.00 | 37.24 | C |
| ATOM | 754 | N | ALA | A | 109 | 27.484 | 31.427 | 50.090 | 1.00 | 34.73 | N |
| ATOM | 755 | CA | ALA | A | 109 | 28.039 | 31.922 | 51.359 | 1.00 | 36.13 | C |
| ATOM | 756 | C | ALA | A | 109 | 28.555 | 33.361 | 51.266 | 1.00 | 37.12 | C |
| ATOM | 757 | O | ALA | A | 109 | 28.455 | 34.127 | 52.213 | 1.00 | 37.35 | O |
| ATOM | 758 | CB | ALA | A | 109 | 29.147 | 30.991 | 51.860 | 1.00 | 35.96 | C |
| ATOM | 759 | N | ASN | A | 110 | 29.076 | 33.745 | 50.112 | 1.00 | 38.70 | N |
| ATOM | 760 | CA | ASN | A | 110 | 29.631 | 35.090 | 49.949 | 1.00 | 39.61 | C |
| ATOM | 761 | C | ASN | A | 110 | 28.605 | 36.188 | 49.621 | 1.00 | 39.61 | C |
| ATOM | 762 | O | ASN | A | 110 | 28.950 | 37.359 | 49.500 | 1.00 | 39.50 | O |
| ATOM | 763 | CB | ASN | A | 110 | 30.730 | 35.036 | 48.888 | 1.00 | 39.94 | C |
| ATOM | 764 | CG | ASN | A | 110 | 31.916 | 34.186 | 49.329 | 1.00 | 41.54 | C |
| ATOM | 765 | OD1 | ASN | A | 110 | 32.341 | 34.223 | 50.503 | 1.00 | 41.36 | O |
| ATOM | 766 | ND2 | ASN | A | 110 | 32.451 | 33.406 | 48.399 | 1.00 | 43.06 | N |
| ATOM | 767 | N | PHE | A | 111 | 27.349 | 35.802 | 49.465 | 1.00 | 40.12 | N |
| ATOM | 768 | CA | PHE | A | 111 | 26.278 | 36.753 | 49.208 | 1.00 | 40.43 | C |
| ATOM | 769 | C | PHE | A | 111 | 25.064 | 36.292 | 50.016 | 1.00 | 41.38 | C |
| ATOM | 770 | O | PHE | A | 111 | 24.068 | 35.811 | 49.471 | 1.00 | 40.89 | O |
| ATOM | 771 | CB | PHE | A | 111 | 25.954 | 36.839 | 47.710 | 1.00 | 40.30 | C |
| ATOM | 772 | CG | PHE | A | 111 | 26.973 | 37.597 | 46.910 | 1.00 | 38.60 | C |
| ATOM | 773 | CD1 | PHE | A | 111 | 28.199 | 37.033 | 46.618 | 1.00 | 37.50 | C |
| ATOM | 774 | CD2 | PHE | A | 111 | 26.705 | 38.867 | 46.445 | 1.00 | 38.02 | C |
| ATOM | 775 | CE1 | PHE | A | 111 | 29.140 | 37.725 | 45.890 | 1.00 | 36.74 | C |
| ATOM | 776 | CE2 | PHE | A | 111 | 27.649 | 39.560 | 45.705 | 1.00 | 36.60 | C |
| ATOM | 777 | CZ | PHE | A | 111 | 28.863 | 38.986 | 45.433 | 1.00 | 35.45 | C |
| ATOM | 778 | N | GLN | A | 112 | 25.175 | 36.457 | 51.329 | 1.00 | 42.72 | N |
| ATOM | 779 | CA | GLN | A | 112 | 24.154 | 36.022 | 52.276 | 1.00 | 43.86 | C |
| ATOM | 780 | C | GLN | A | 112 | 22.790 | 36.598 | 51.948 | 1.00 | 44.00 | C |
| ATOM | 781 | O | GLN | A | 112 | 21.774 | 35.994 | 52.280 | 1.00 | 44.39 | O |
| ATOM | 782 | CB | GLN | A | 112 | 24.535 | 36.428 | 53.706 | 1.00 | 44.29 | C |
| ATOM | 783 | CG | GLN | A | 112 | 25.923 | 35.985 | 54.166 | 1.00 | 46.45 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 784 | CD | GLN | A | 112 | 26.050 | 34.477 | 54.296 | 1.00 | 49.14 | C |
| ATOM | 785 | OE1 | GLN | A | 112 | 25.523 | 33.733 | 53.466 | 1.00 | 50.83 | O |
| ATOM | 786 | NE2 | GLN | A | 112 | 26.756 | 34.022 | 55.332 | 1.00 | 50.52 | N |
| ATOM | 787 | N | ASN | A | 113 | 22.765 | 37.759 | 51.299 | 1.00 | 43.96 | N |
| ATOM | 788 | CA | ASN | A | 113 | 21.504 | 38.416 | 50.971 | 1.00 | 44.15 | C |
| ATOM | 789 | C | ASN | A | 113 | 20.827 | 37.921 | 49.679 | 1.00 | 44.12 | C |
| ATOM | 790 | O | ASN | A | 113 | 19.768 | 38.431 | 49.309 | 1.00 | 44.11 | O |
| ATOM | 791 | CB | ASN | A | 113 | 21.696 | 39.941 | 50.918 | 1.00 | 44.21 | C |
| ATOM | 792 | CG | ASN | A | 113 | 22.084 | 40.541 | 52.283 | 1.00 | 44.80 | C |
| ATOM | 793 | OD1 | ASN | A | 113 | 21.759 | 39.991 | 53.349 | 1.00 | 43.65 | O |
| ATOM | 794 | ND2 | ASN | A | 113 | 22.778 | 41.675 | 52.246 | 1.00 | 44.92 | N |
| ATOM | 795 | N | PHE | A | 114 | 21.415 | 36.939 | 48.995 | 1.00 | 43.98 | N |
| ATOM | 796 | CA | PHE | A | 114 | 20.793 | 36.411 | 47.787 | 1.00 | 43.71 | C |
| ATOM | 797 | C | PHE | A | 114 | 19.778 | 35.345 | 48.150 | 1.00 | 43.76 | C |
| ATOM | 798 | O | PHE | A | 114 | 20.111 | 34.362 | 48.815 | 1.00 | 43.32 | O |
| ATOM | 799 | CB | PHE | A | 114 | 21.813 | 35.808 | 46.833 | 1.00 | 43.82 | C |
| ATOM | 800 | CG | PHE | A | 114 | 21.184 | 35.128 | 45.650 | 1.00 | 43.80 | C |
| ATOM | 801 | CD1 | PHE | A | 114 | 20.567 | 35.881 | 44.661 | 1.00 | 43.54 | C |
| ATOM | 802 | CD2 | PHE | A | 114 | 21.170 | 33.745 | 45.541 | 1.00 | 43.65 | C |
| ATOM | 803 | CE1 | PHE | A | 114 | 19.963 | 35.276 | 43.587 | 1.00 | 43.55 | C |
| ATOM | 804 | CE2 | PHE | A | 114 | 20.566 | 33.129 | 44.451 | 1.00 | 43.21 | C |
| ATOM | 805 | CZ | PHE | A | 114 | 19.961 | 33.897 | 43.476 | 1.00 | 42.89 | C |
| ATOM | 806 | N | LYS | A | 115 | 18.543 | 35.543 | 47.705 | 1.00 | 43.96 | N |
| ATOM | 807 | CA | LYS | A | 115 | 17.459 | 34.613 | 47.999 | 1.00 | 44.38 | C |
| ATOM | 808 | C | LYS | A | 115 | 16.933 | 34.026 | 46.693 | 1.00 | 44.04 | C |
| ATOM | 809 | O | LYS | A | 115 | 16.213 | 34.687 | 45.945 | 1.00 | 43.97 | O |
| ATOM | 810 | CB | LYS | A | 115 | 16.342 | 35.329 | 48.761 | 1.00 | 44.79 | C |
| ATOM | 811 | CG | LYS | A | 115 | 16.763 | 35.866 | 50.129 | 1.00 | 46.74 | C |
| ATOM | 812 | CD | LYS | A | 115 | 17.021 | 34.744 | 51.130 | 1.00 | 48.83 | C |
| ATOM | 813 | CE | LYS | A | 115 | 17.461 | 35.288 | 52.484 | 1.00 | 50.18 | C |
| ATOM | 814 | NZ | LYS | A | 115 | 17.498 | 34.224 | 53.539 | 1.00 | 51.05 | N |
| ATOM | 815 | N | PRO | A | 116 | 17.270 | 32.771 | 46.433 | 1.00 | 43.65 | N |
| ATOM | 816 | CA | PRO | A | 116 | 16.918 | 32.133 | 45.160 | 1.00 | 43.43 | C |
| ATOM | 817 | C | PRO | A | 116 | 15.415 | 32.034 | 44.969 | 1.00 | 42.76 | C |
| ATOM | 818 | O | PRO | A | 116 | 14.711 | 31.724 | 45.915 | 1.00 | 42.78 | O |
| ATOM | 819 | CB | PRO | A | 116 | 17.525 | 30.732 | 45.273 | 1.00 | 43.57 | C |
| ATOM | 820 | CG | PRO | A | 116 | 18.385 | 30.743 | 46.496 | 1.00 | 43.88 | C |
| ATOM | 821 | CD | PRO | A | 116 | 17.948 | 31.855 | 47.359 | 1.00 | 43.68 | C |
| ATOM | 822 | N | ARG | A | 117 | 14.940 | 32.306 | 43.761 | 1.00 | 42.20 | N |
| ATOM | 823 | CA | ARG | A | 117 | 13.518 | 32.214 | 43.451 | 1.00 | 41.56 | C |
| ATOM | 824 | C | ARG | A | 117 | 13.140 | 30.780 | 43.104 | 1.00 | 41.00 | C |
| ATOM | 825 | O | ARG | A | 117 | 11.957 | 30.461 | 43.007 | 1.00 | 41.15 | O |
| ATOM | 826 | CB | ARG | A | 117 | 13.164 | 33.132 | 42.311 | 1.00 | 41.47 | C |
| ATOM | 827 | N | SER | A | 118 | 14.139 | 29.925 | 42.904 | 1.00 | 40.00 | N |
| ATOM | 828 | CA | SER | A | 118 | 13.882 | 28.517 | 42.654 | 1.00 | 39.60 | C |
| ATOM | 829 | C | SER | A | 118 | 14.700 | 27.655 | 43.621 | 1.00 | 39.30 | C |
| ATOM | 830 | O | SER | A | 118 | 15.756 | 28.078 | 44.087 | 1.00 | 39.24 | O |
| ATOM | 831 | CB | SER | A | 118 | 14.184 | 28.158 | 41.196 | 1.00 | 39.30 | C |
| ATOM | 832 | OG | SER | A | 118 | 15.560 | 28.228 | 40.942 | 1.00 | 38.53 | O |
| ATOM | 833 | N | ASN | A | 119 | 14.180 | 26.471 | 43.943 | 1.00 | 38.96 | N |
| ATOM | 834 | CA | ASN | A | 119 | 14.838 | 25.537 | 44.854 | 1.00 | 38.95 | C |
| ATOM | 835 | C | ASN | A | 119 | 15.115 | 24.215 | 44.160 | 1.00 | 37.99 | C |
| ATOM | 836 | O | ASN | A | 119 | 14.314 | 23.751 | 43.359 | 1.00 | 37.35 | O |
| ATOM | 837 | CB | ASN | A | 119 | 13.958 | 25.220 | 46.068 | 1.00 | 39.54 | C |
| ATOM | 838 | CG | ASN | A | 119 | 13.466 | 26.456 | 46.797 | 1.00 | 41.82 | C |
| ATOM | 839 | OD1 | ASN | A | 119 | 14.255 | 27.279 | 47.289 | 1.00 | 44.50 | O |
| ATOM | 840 | ND2 | ASN | A | 119 | 12.145 | 26.574 | 46.906 | 1.00 | 44.99 | N |
| ATOM | 841 | N | ARG | A | 120 | 16.243 | 23.607 | 44.492 | 1.00 | 37.46 | N |
| ATOM | 842 | CA | ARG | A | 120 | 16.627 | 22.325 | 43.927 | 1.00 | 37.15 | C |
| ATOM | 843 | C | ARG | A | 120 | 16.209 | 21.193 | 44.844 | 1.00 | 37.03 | C |
| ATOM | 844 | O | ARG | A | 120 | 16.359 | 21.272 | 46.069 | 1.00 | 37.28 | O |

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ATOM    845  CB  ARG A 120      18.144  22.264  43.730  1.00 37.07           C
ATOM    846  CG  ARG A 120      18.632  21.020  42.993  1.00 36.32           C
ATOM    847  CD  ARG A 120      20.152  20.886  42.938  1.00 35.46           C
ATOM    848  NE  ARG A 120      20.777  21.277  44.198  1.00 34.29           N
ATOM    849  CZ  ARG A 120      21.049  20.445  45.202  1.00 36.66           C
ATOM    850  NH1 ARG A 120      20.753  19.147  45.122  1.00 35.60           N
ATOM    851  NH2 ARG A 120      21.614  20.915  46.305  1.00 37.13           N
ATOM    852  N   GLU A 121      15.665  20.141  44.250  1.00 36.76           N
ATOM    853  CA  GLU A 121      15.326  18.944  44.993  1.00 36.29           C
ATOM    854  C   GLU A 121      15.810  17.746  44.187  1.00 35.35           C
ATOM    855  O   GLU A 121      15.709  17.726  42.953  1.00 35.38           O
ATOM    856  CB  GLU A 121      13.820  18.863  45.262  1.00 36.78           C
ATOM    857  CG  GLU A 121      13.398  17.585  45.971  1.00 39.29           C
ATOM    858  CD  GLU A 121      12.126  17.732  46.795  1.00 42.09           C
ATOM    859  OE1 GLU A 121      12.200  18.310  47.904  1.00 45.56           O
ATOM    860  OE2 GLU A 121      11.059  17.254  46.350  1.00 43.04           O
ATOM    861  N   GLU A 122      16.366  16.764  44.886  1.00 34.04           N
ATOM    862  CA  GLU A 122      16.840  15.547  44.266  1.00 33.04           C
ATOM    863  C   GLU A 122      15.748  14.518  44.415  1.00 32.55           C
ATOM    864  O   GLU A 122      15.253  14.306  45.511  1.00 32.52           O
ATOM    865  CB  GLU A 122      18.103  15.052  44.961  1.00 32.71           C
ATOM    866  CG  GLU A 122      19.265  16.018  44.885  1.00 31.86           C
ATOM    867  CD  GLU A 122      19.705  16.296  43.454  1.00 31.04           C
ATOM    868  OE1 GLU A 122      20.065  15.331  42.757  1.00 29.68           O
ATOM    869  OE2 GLU A 122      19.694  17.479  43.025  1.00 29.20           O
ATOM    870  N   MET A 123      15.349  13.885  43.321  1.00 31.83           N
ATOM    871  CA  MET A 123      14.329  12.858  43.415  1.00 31.40           C
ATOM    872  C   MET A 123      14.532  11.820  42.343  1.00 30.68           C
ATOM    873  O   MET A 123      15.380  11.982  41.457  1.00 30.07           O
ATOM    874  CB  MET A 123      12.931  13.466  43.309  1.00 31.52           C
ATOM    875  CG  MET A 123      12.667  14.205  42.032  1.00 32.93           C
ATOM    876  SD  MET A 123      11.115  15.145  42.034  1.00 35.27           S
ATOM    877  CE  MET A 123      11.554  16.565  42.966  1.00 35.33           C
ATOM    878  N   LYS A 124      13.766  10.738  42.464  1.00 29.85           N
ATOM    879  CA  LYS A 124      13.752   9.671  41.483  1.00 29.22           C
ATOM    880  C   LYS A 124      12.891  10.140  40.307  1.00 28.45           C
ATOM    881  O   LYS A 124      12.066  11.039  40.466  1.00 27.39           O
ATOM    882  CB  LYS A 124      13.183   8.389  42.100  1.00 29.57           C
ATOM    883  CG  LYS A 124      13.954   7.857  43.321  1.00 29.88           C
ATOM    884  CD  LYS A 124      15.392   7.501  42.950  1.00 30.48           C
ATOM    885  CE  LYS A 124      16.231   7.129  44.167  1.00 30.33           C
ATOM    886  NZ  LYS A 124      17.691   7.276  43.872  1.00 30.47           N
ATOM    887  N   PHE A 125      13.075   9.536  39.133  1.00 27.71           N
ATOM    888  CA  PHE A 125      12.364  10.000  37.949  1.00 27.22           C
ATOM    889  C   PHE A 125      10.869   9.891  38.114  1.00 27.29           C
ATOM    890  O   PHE A 125      10.138  10.825  37.801  1.00 26.75           O
ATOM    891  CB  PHE A 125      12.794   9.270  36.681  1.00 26.90           C
ATOM    892  CG  PHE A 125      12.494  10.051  35.433  1.00 27.63           C
ATOM    893  CD1 PHE A 125      13.330  11.083  35.032  1.00 27.70           C
ATOM    894  CD2 PHE A 125      11.351   9.802  34.702  1.00 28.29           C
ATOM    895  CE1 PHE A 125      13.059  11.828  33.905  1.00 27.96           C
ATOM    896  CE2 PHE A 125      11.065  10.540  33.563  1.00 29.16           C
ATOM    897  CZ  PHE A 125      11.924  11.568  33.167  1.00 28.71           C
ATOM    898  N   HIS A 126      10.426   8.743  38.620  1.00 27.46           N
ATOM    899  CA  HIS A 126       9.013   8.499  38.832  1.00 27.77           C
ATOM    900  C   HIS A 126       8.430   9.522  39.794  1.00 27.71           C
ATOM    901  O   HIS A 126       7.245   9.821  39.731  1.00 27.27           O
ATOM    902  CB  HIS A 126       8.770   7.056  39.329  1.00 27.96           C
ATOM    903  CG  HIS A 126       8.897   6.880  40.812  1.00 28.47           C
ATOM    904  ND1 HIS A 126       7.831   7.026  41.672  1.00 29.29           N
ATOM    905  CD2 HIS A 126       9.961   6.552  41.585  1.00 29.43           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 906 | CE1 | HIS | A | 126 | 8.236 | 6.812 | 42.912 | 1.00 | 30.26 | C |
| ATOM | 907 | NE2 | HIS | A | 126 | 9.525 | 6.524 | 42.887 | 1.00 | 29.64 | N |
| ATOM | 908 | N | GLU | A | 127 | 9.262 | 10.059 | 40.679 | 1.00 | 28.09 | N |
| ATOM | 909 | CA | GLU | A | 127 | 8.803 | 11.078 | 41.615 | 1.00 | 28.68 | C |
| ATOM | 910 | C | GLU | A | 127 | 8.585 | 12.400 | 40.865 | 1.00 | 28.99 | C |
| ATOM | 911 | O | GLU | A | 127 | 7.626 | 13.129 | 41.123 | 1.00 | 29.15 | O |
| ATOM | 912 | CB | GLU | A | 127 | 9.795 | 11.233 | 42.775 | 1.00 | 28.52 | C |
| ATOM | 913 | CG | GLU | A | 127 | 9.931 | 9.968 | 43.626 | 1.00 | 29.84 | C |
| ATOM | 914 | CD | GLU | A | 127 | 10.873 | 10.121 | 44.810 | 1.00 | 30.26 | C |
| ATOM | 915 | OE1 | GLU | A | 127 | 12.069 | 10.398 | 44.603 | 1.00 | 29.68 | O |
| ATOM | 916 | OE2 | GLU | A | 127 | 10.410 | 9.943 | 45.962 | 1.00 | 32.95 | O |
| ATOM | 917 | N | PHE | A | 128 | 9.471 | 12.696 | 39.927 | 1.00 | 29.39 | N |
| ATOM | 918 | CA | PHE | A | 128 | 9.354 | 13.914 | 39.119 | 1.00 | 29.64 | C |
| ATOM | 919 | C | PHE | A | 128 | 8.047 | 13.859 | 38.333 | 1.00 | 30.31 | C |
| ATOM | 920 | O | PHE | A | 128 | 7.274 | 14.817 | 38.294 | 1.00 | 29.97 | O |
| ATOM | 921 | CB | PHE | A | 128 | 10.551 | 14.017 | 38.167 | 1.00 | 29.10 | C |
| ATOM | 922 | CG | PHE | A | 128 | 10.337 | 14.950 | 36.991 | 1.00 | 28.33 | C |
| ATOM | 923 | CD1 | PHE | A | 128 | 10.106 | 16.301 | 37.188 | 1.00 | 26.53 | C |
| ATOM | 924 | CD2 | PHE | A | 128 | 10.397 | 14.475 | 35.696 | 1.00 | 26.99 | C |
| ATOM | 925 | CE1 | PHE | A | 128 | 9.920 | 17.149 | 36.120 | 1.00 | 27.50 | C |
| ATOM | 926 | CE2 | PHE | A | 128 | 10.217 | 15.341 | 34.610 | 1.00 | 28.49 | C |
| ATOM | 927 | CZ | PHE | A | 128 | 9.976 | 16.668 | 34.823 | 1.00 | 26.78 | C |
| ATOM | 928 | N | VAL | A | 129 | 7.797 | 12.705 | 37.736 | 1.00 | 31.32 | N |
| ATOM | 929 | CA | VAL | A | 129 | 6.603 | 12.499 | 36.930 | 1.00 | 32.38 | C |
| ATOM | 930 | C | VAL | A | 129 | 5.338 | 12.658 | 37.775 | 1.00 | 32.96 | C |
| ATOM | 931 | O | VAL | A | 129 | 4.398 | 13.362 | 37.388 | 1.00 | 32.79 | O |
| ATOM | 932 | CB | VAL | A | 129 | 6.606 | 11.094 | 36.313 | 1.00 | 32.48 | C |
| ATOM | 933 | CG1 | VAL | A | 129 | 5.313 | 10.840 | 35.551 | 1.00 | 32.96 | C |
| ATOM | 934 | CG2 | VAL | A | 129 | 7.828 | 10.901 | 35.417 | 1.00 | 31.98 | C |
| ATOM | 935 | N | GLU | A | 130 | 5.329 | 11.993 | 38.925 | 1.00 | 33.61 | N |
| ATOM | 936 | CA | GLU | A | 130 | 4.205 | 12.067 | 39.853 | 1.00 | 34.29 | C |
| ATOM | 937 | C | GLU | A | 130 | 3.963 | 13.515 | 40.246 | 1.00 | 34.51 | C |
| ATOM | 938 | O | GLU | A | 130 | 2.832 | 13.986 | 40.220 | 1.00 | 33.80 | O |
| ATOM | 939 | CB | GLU | A | 130 | 4.481 | 11.206 | 41.087 | 1.00 | 34.35 | C |
| ATOM | 940 | CG | GLU | A | 130 | 4.372 | 9.711 | 40.815 | 1.00 | 34.92 | C |
| ATOM | 941 | CD | GLU | A | 130 | 5.204 | 8.858 | 41.761 | 1.00 | 35.66 | C |
| ATOM | 942 | OE1 | GLU | A | 130 | 5.595 | 9.345 | 42.845 | 1.00 | 36.55 | O |
| ATOM | 943 | OE2 | GLU | A | 130 | 5.477 | 7.692 | 41.407 | 1.00 | 36.06 | O |
| ATOM | 944 | N | LYS | A | 131 | 5.033 | 14.223 | 40.587 | 1.00 | 35.27 | N |
| ATOM | 945 | CA | LYS | A | 131 | 4.912 | 15.632 | 40.920 | 1.00 | 36.15 | C |
| ATOM | 946 | C | LYS | A | 131 | 4.286 | 16.408 | 39.758 | 1.00 | 36.63 | C |
| ATOM | 947 | O | LYS | A | 131 | 3.420 | 17.253 | 39.972 | 1.00 | 36.42 | O |
| ATOM | 948 | CB | LYS | A | 131 | 6.269 | 16.240 | 41.261 | 1.00 | 36.51 | C |
| ATOM | 949 | CG | LYS | A | 131 | 6.467 | 16.623 | 42.712 | 1.00 | 37.67 | C |
| ATOM | 950 | CD | LYS | A | 131 | 7.125 | 18.001 | 42.822 | 1.00 | 38.95 | C |
| ATOM | 951 | CE | LYS | A | 131 | 7.581 | 18.324 | 44.252 | 1.00 | 40.39 | C |
| ATOM | 952 | NZ | LYS | A | 131 | 8.073 | 19.747 | 44.404 | 1.00 | 40.82 | N |
| ATOM | 953 | N | LEU | A | 132 | 4.725 | 16.142 | 38.532 | 1.00 | 37.30 | N |
| ATOM | 954 | CA | LEU | A | 132 | 4.156 | 16.845 | 37.383 | 1.00 | 38.29 | C |
| ATOM | 955 | C | LEU | A | 132 | 2.669 | 16.557 | 37.280 | 1.00 | 38.83 | C |
| ATOM | 956 | O | LEU | A | 132 | 1.875 | 17.449 | 36.976 | 1.00 | 38.56 | O |
| ATOM | 957 | CB | LEU | A | 132 | 4.819 | 16.424 | 36.081 | 1.00 | 38.42 | C |
| ATOM | 958 | CG | LEU | A | 132 | 6.224 | 16.916 | 35.791 | 1.00 | 39.15 | C |
| ATOM | 959 | CD1 | LEU | A | 132 | 6.671 | 16.296 | 34.485 | 1.00 | 39.76 | C |
| ATOM | 960 | CD2 | LEU | A | 132 | 6.281 | 18.433 | 35.712 | 1.00 | 39.81 | C |
| ATOM | 961 | N | GLN | A | 133 | 2.311 | 15.300 | 37.529 | 1.00 | 39.68 | N |
| ATOM | 962 | CA | GLN | A | 133 | 0.920 | 14.863 | 37.495 | 1.00 | 40.45 | C |
| ATOM | 963 | C | GLN | A | 133 | 0.057 | 15.580 | 38.541 | 1.00 | 41.05 | C |
| ATOM | 964 | O | GLN | A | 133 | -1.035 | 16.040 | 38.222 | 1.00 | 41.20 | O |
| ATOM | 965 | CB | GLN | A | 133 | 0.835 | 13.344 | 37.681 | 1.00 | 40.31 | C |
| ATOM | 966 | N | ASP | A | 134 | 0.542 | 15.682 | 39.777 | 1.00 | 41.89 | N |

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ATOM    967  CA  ASP A 134      -0.232  16.313  40.854  1.00 42.72           C
ATOM    968  C   ASP A 134      -0.506  17.792  40.576  1.00 42.60           C
ATOM    969  O   ASP A 134      -1.570  18.316  40.900  1.00 42.25           O
ATOM    970  CB  ASP A 134       0.491  16.169  42.200  1.00 43.21           C
ATOM    971  CG  ASP A 134      -0.429  16.419  43.396  1.00 45.71           C
ATOM    972  OD1 ASP A 134      -1.566  16.916  43.213  1.00 48.39           O
ATOM    973  OD2 ASP A 134      -0.104  16.131  44.571  1.00 49.60           O
ATOM    974  N   ILE A 135       0.467  18.467  39.981  1.00 42.77           N
ATOM    975  CA  ILE A 135       0.306  19.872  39.660  1.00 42.91           C
ATOM    976  C   ILE A 135      -0.793  20.050  38.626  1.00 43.15           C
ATOM    977  O   ILE A 135      -1.690  20.871  38.800  1.00 43.03           O
ATOM    978  CB  ILE A 135       1.623  20.443  39.155  1.00 42.94           C
ATOM    979  CG1 ILE A 135       2.586  20.607  40.330  1.00 43.10           C
ATOM    980  CG2 ILE A 135       1.396  21.778  38.473  1.00 42.80           C
ATOM    981  CD1 ILE A 135       4.040  20.621  39.934  1.00 43.49           C
ATOM    982  N   GLN A 136      -0.716  19.272  37.554  1.00 43.64           N
ATOM    983  CA  GLN A 136      -1.712  19.321  36.496  1.00 44.17           C
ATOM    984  C   GLN A 136      -3.103  19.129  37.081  1.00 44.65           C
ATOM    985  O   GLN A 136      -3.976  19.984  36.936  1.00 44.71           O
ATOM    986  CB  GLN A 136      -1.431  18.240  35.466  1.00 44.19           C
ATOM    987  N   GLN A 137      -3.289  18.014  37.776  1.00 45.23           N
ATOM    988  CA  GLN A 137      -4.596  17.654  38.314  1.00 45.66           C
ATOM    989  C   GLN A 137      -5.146  18.696  39.277  1.00 45.88           C
ATOM    990  O   GLN A 137      -6.337  19.005  39.238  1.00 46.33           O
ATOM    991  CB  GLN A 137      -4.535  16.277  38.991  1.00 45.74           C
ATOM    992  N   ARG A 138      -4.288  19.246  40.131  1.00 45.93           N
ATOM    993  CA  ARG A 138      -4.740  20.211  41.132  1.00 45.84           C
ATOM    994  C   ARG A 138      -4.720  21.640  40.592  1.00 45.53           C
ATOM    995  O   ARG A 138      -4.911  22.598  41.344  1.00 45.72           O
ATOM    996  CB  ARG A 138      -3.880  20.108  42.398  1.00 45.92           C
ATOM    997  CG  ARG A 138      -2.551  20.866  42.340  1.00 46.84           C
ATOM    998  CD  ARG A 138      -1.589  20.458  43.437  1.00 47.70           C
ATOM    999  NE  ARG A 138      -0.509  21.418  43.652  1.00 47.78           N
ATOM   1000  CZ  ARG A 138       0.788  21.125  43.578  1.00 49.17           C
ATOM   1001  NH1 ARG A 138       1.186  19.897  43.274  1.00 50.12           N
ATOM   1002  NH2 ARG A 138       1.702  22.064  43.798  1.00 49.52           N
ATOM   1003  N   GLY A 139      -4.492  21.783  39.290  1.00 44.99           N
ATOM   1004  CA  GLY A 139      -4.419  23.094  38.669  1.00 44.52           C
ATOM   1005  C   GLY A 139      -3.412  24.041  39.310  1.00 44.06           C
ATOM   1006  O   GLY A 139      -3.551  25.259  39.203  1.00 44.28           O
ATOM   1007  N   GLY A 140      -2.382  23.495  39.953  1.00 43.28           N
ATOM   1008  CA  GLY A 140      -1.388  24.309  40.629  1.00 42.49           C
ATOM   1009  C   GLY A 140      -0.609  25.218  39.694  1.00 41.92           C
ATOM   1010  O   GLY A 140      -0.556  24.989  38.480  1.00 41.85           O
ATOM   1011  N   GLU A 141      -0.004  26.264  40.250  1.00 40.90           N
ATOM   1012  CA  GLU A 141       0.789  27.186  39.444  1.00 40.07           C
ATOM   1013  C   GLU A 141       2.286  26.884  39.549  1.00 38.68           C
ATOM   1014  O   GLU A 141       3.096  27.503  38.867  1.00 38.67           O
ATOM   1015  CB  GLU A 141       0.513  28.644  39.839  1.00 40.36           C
ATOM   1016  CG  GLU A 141      -0.799  29.224  39.309  1.00 41.91           C
ATOM   1017  CD  GLU A 141      -1.001  29.042  37.805  1.00 44.25           C
ATOM   1018  OE1 GLU A 141       0.004  29.008  37.043  1.00 45.69           O
ATOM   1019  OE2 GLU A 141      -2.181  28.940  37.380  1.00 44.55           O
ATOM   1020  N   GLU A 142       2.648  25.944  40.413  1.00 37.02           N
ATOM   1021  CA  GLU A 142       4.040  25.573  40.596  1.00 35.61           C
ATOM   1022  C   GLU A 142       4.629  25.120  39.265  1.00 34.41           C
ATOM   1023  O   GLU A 142       3.923  24.594  38.408  1.00 34.25           O
ATOM   1024  CB  GLU A 142       4.150  24.443  41.627  1.00 35.49           C
ATOM   1025  CG  GLU A 142       5.571  24.173  42.095  1.00 35.47           C
ATOM   1026  CD  GLU A 142       5.710  22.944  42.978  1.00 36.48           C
ATOM   1027  OE1 GLU A 142       4.733  22.174  43.142  1.00 37.45           O
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1028 | OE2 | GLU | A | 142 | 6.821 | 22.739 | 43.511 | 1.00 | 36.76 | O |
| ATOM | 1029 | N | ARG | A | 143 | 5.926 | 25.323 | 39.096 | 1.00 | 32.91 | N |
| ATOM | 1030 | CA | ARG | A | 143 | 6.596 | 24.893 | 37.884 | 1.00 | 31.95 | C |
| ATOM | 1031 | C | ARG | A | 143 | 7.803 | 24.058 | 38.214 | 1.00 | 30.62 | C |
| ATOM | 1032 | O | ARG | A | 143 | 8.514 | 24.354 | 39.166 | 1.00 | 30.75 | O |
| ATOM | 1033 | CB | ARG | A | 143 | 7.072 | 26.097 | 37.082 | 1.00 | 32.19 | C |
| ATOM | 1034 | CG | ARG | A | 143 | 5.968 | 26.912 | 36.447 | 1.00 | 32.57 | C |
| ATOM | 1035 | CD | ARG | A | 143 | 6.507 | 28.170 | 35.801 | 1.00 | 32.53 | C |
| ATOM | 1036 | NE | ARG | A | 143 | 5.492 | 28.885 | 35.037 | 1.00 | 32.25 | N |
| ATOM | 1037 | CZ | ARG | A | 143 | 5.158 | 28.617 | 33.790 | 1.00 | 31.80 | C |
| ATOM | 1038 | NH1 | ARG | A | 143 | 5.757 | 27.637 | 33.105 | 1.00 | 31.28 | N |
| ATOM | 1039 | NH2 | ARG | A | 143 | 4.214 | 29.345 | 33.221 | 1.00 | 32.77 | N |
| ATOM | 1040 | N | LEU | A | 144 | 8.054 | 23.028 | 37.417 | 1.00 | 28.97 | N |
| ATOM | 1041 | CA | LEU | A | 144 | 9.235 | 22.219 | 37.617 | 1.00 | 28.09 | C |
| ATOM | 1042 | C | LEU | A | 144 | 10.150 | 22.257 | 36.398 | 1.00 | 27.14 | C |
| ATOM | 1043 | O | LEU | A | 144 | 9.690 | 22.418 | 35.272 | 1.00 | 26.74 | O |
| ATOM | 1044 | CB | LEU | A | 144 | 8.834 | 20.783 | 37.887 | 1.00 | 28.28 | C |
| ATOM | 1045 | CG | LEU | A | 144 | 7.839 | 20.606 | 39.038 | 1.00 | 28.89 | C |
| ATOM | 1046 | CD1 | LEU | A | 144 | 7.515 | 19.123 | 39.216 | 1.00 | 29.62 | C |
| ATOM | 1047 | CD2 | LEU | A | 144 | 8.364 | 21.212 | 40.333 | 1.00 | 27.84 | C |
| ATOM | 1048 | N | TYR | A | 145 | 11.447 | 22.102 | 36.636 | 1.00 | 25.69 | N |
| ATOM | 1049 | CA | TYR | A | 145 | 12.395 | 21.976 | 35.548 | 1.00 | 25.05 | C |
| ATOM | 1050 | C | TYR | A | 145 | 13.459 | 20.957 | 35.968 | 1.00 | 25.00 | C |
| ATOM | 1051 | O | TYR | A | 145 | 14.239 | 21.193 | 36.881 | 1.00 | 25.01 | O |
| ATOM | 1052 | CB | TYR | A | 145 | 13.022 | 23.327 | 35.183 | 1.00 | 24.76 | C |
| ATOM | 1053 | CG | TYR | A | 145 | 13.471 | 23.485 | 33.728 | 1.00 | 23.25 | C |
| ATOM | 1054 | CD1 | TYR | A | 145 | 13.739 | 22.385 | 32.931 | 1.00 | 21.70 | C |
| ATOM | 1055 | CD2 | TYR | A | 145 | 13.667 | 24.746 | 33.175 | 1.00 | 22.16 | C |
| ATOM | 1056 | CE1 | TYR | A | 145 | 14.154 | 22.526 | 31.620 | 1.00 | 20.98 | C |
| ATOM | 1057 | CE2 | TYR | A | 145 | 14.097 | 24.904 | 31.846 | 1.00 | 21.30 | C |
| ATOM | 1058 | CZ | TYR | A | 145 | 14.332 | 23.799 | 31.071 | 1.00 | 20.66 | C |
| ATOM | 1059 | OH | TYR | A | 145 | 14.737 | 23.933 | 29.740 | 1.00 | 18.41 | O |
| ATOM | 1060 | N | LEU | A | 146 | 13.446 | 19.808 | 35.318 | 1.00 | 24.95 | N |
| ATOM | 1061 | CA | LEU | A | 146 | 14.453 | 18.787 | 35.547 | 1.00 | 25.43 | C |
| ATOM | 1062 | C | LEU | A | 146 | 15.678 | 19.100 | 34.694 | 1.00 | 24.91 | C |
| ATOM | 1063 | O | LEU | A | 146 | 15.555 | 19.313 | 33.493 | 1.00 | 24.10 | O |
| ATOM | 1064 | CB | LEU | A | 146 | 13.907 | 17.419 | 35.162 | 1.00 | 25.59 | C |
| ATOM | 1065 | CG | LEU | A | 146 | 14.875 | 16.238 | 35.334 | 1.00 | 27.52 | C |
| ATOM | 1066 | CD1 | LEU | A | 146 | 14.111 | 14.966 | 35.672 | 1.00 | 26.95 | C |
| ATOM | 1067 | CD2 | LEU | A | 146 | 15.742 | 16.023 | 34.084 | 1.00 | 29.46 | C |
| ATOM | 1068 | N | GLN | A | 147 | 16.845 | 19.097 | 35.330 | 1.00 | 24.91 | N |
| ATOM | 1069 | CA | GLN | A | 147 | 18.115 | 19.394 | 34.685 | 1.00 | 25.27 | C |
| ATOM | 1070 | C | GLN | A | 147 | 19.146 | 18.490 | 35.317 | 1.00 | 25.28 | C |
| ATOM | 1071 | O | GLN | A | 147 | 19.610 | 18.740 | 36.419 | 1.00 | 27.14 | O |
| ATOM | 1072 | CB | GLN | A | 147 | 18.475 | 20.876 | 34.863 | 1.00 | 25.02 | C |
| ATOM | 1073 | CG | GLN | A | 147 | 17.321 | 21.804 | 34.485 | 1.00 | 24.97 | C |
| ATOM | 1074 | CD | GLN | A | 147 | 17.682 | 23.283 | 34.560 | 1.00 | 27.08 | C |
| ATOM | 1075 | OE1 | GLN | A | 147 | 16.891 | 24.149 | 34.141 | 1.00 | 27.93 | O |
| ATOM | 1076 | NE2 | GLN | A | 147 | 18.860 | 23.575 | 35.064 | 1.00 | 23.50 | N |
| ATOM | 1077 | N | GLN | A | 148 | 19.487 | 17.428 | 34.611 | 1.00 | 25.47 | N |
| ATOM | 1078 | CA | GLN | A | 148 | 20.319 | 16.365 | 35.146 | 1.00 | 25.45 | C |
| ATOM | 1079 | C | GLN | A | 148 | 21.254 | 15.816 | 34.105 | 1.00 | 25.50 | C |
| ATOM | 1080 | O | GLN | A | 148 | 20.862 | 15.485 | 32.992 | 1.00 | 25.04 | O |
| ATOM | 1081 | CB | GLN | A | 148 | 19.436 | 15.231 | 35.640 | 1.00 | 25.37 | C |
| ATOM | 1082 | CG | GLN | A | 148 | 20.201 | 14.021 | 36.167 | 1.00 | 26.15 | C |
| ATOM | 1083 | CD | GLN | A | 148 | 21.129 | 14.383 | 37.314 | 1.00 | 26.56 | C |
| ATOM | 1084 | OE1 | GLN | A | 148 | 20.718 | 15.093 | 38.240 | 1.00 | 23.94 | O |
| ATOM | 1085 | NE2 | GLN | A | 148 | 22.383 | 13.916 | 37.248 | 1.00 | 25.29 | N |
| ATOM | 1086 | N | THR | A | 149 | 22.510 | 15.769 | 34.482 | 1.00 | 25.86 | N |
| ATOM | 1087 | CA | THR | A | 149 | 23.552 | 15.219 | 33.667 | 1.00 | 27.04 | C |
| ATOM | 1088 | C | THR | A | 149 | 23.298 | 13.720 | 33.527 | 1.00 | 27.25 | C |

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ATOM   1089  O   THR A 149      23.012  13.044  34.508  1.00 26.86           O
ATOM   1090  CB  THR A 149      24.903  15.540  34.375  1.00 27.42           C
ATOM   1091  OG1 THR A 149      25.300  16.882  34.020  1.00 29.80           O
ATOM   1092  CG2 THR A 149      26.034  14.702  33.873  1.00 28.98           C
ATOM   1093  N   LEU A 150      23.338  13.224  32.298  1.00 27.70           N
ATOM   1094  CA  LEU A 150      23.195  11.812  32.027  1.00 28.46           C
ATOM   1095  C   LEU A 150      24.429  11.076  32.573  1.00 28.97           C
ATOM   1096  O   LEU A 150      25.548  11.468  32.268  1.00 29.00           O
ATOM   1097  CB  LEU A 150      23.084  11.580  30.524  1.00 28.34           C
ATOM   1098  CG  LEU A 150      21.780  11.981  29.837  1.00 29.63           C
ATOM   1099  CD1 LEU A 150      21.944  11.862  28.328  1.00 30.03           C
ATOM   1100  CD2 LEU A 150      20.619  11.140  30.310  1.00 31.15           C
ATOM   1101  N   ASN A 151      24.230  10.030  33.378  1.00 29.35           N
ATOM   1102  CA  ASN A 151      25.348   9.258  33.949  1.00 29.51           C
ATOM   1103  C   ASN A 151      25.137   7.732  33.934  1.00 29.92           C
ATOM   1104  O   ASN A 151      24.162   7.241  33.348  1.00 29.73           O
ATOM   1105  CB  ASN A 151      25.590   9.710  35.385  1.00 29.78           C
ATOM   1106  CG  ASN A 151      24.362   9.553  36.241  1.00 29.19           C
ATOM   1107  OD1 ASN A 151      23.735   8.497  36.260  1.00 30.09           O
ATOM   1108  ND2 ASN A 151      23.991  10.611  36.930  1.00 29.31           N
ATOM   1109  N   ASP A 152      26.020   6.999  34.627  1.00 30.27           N
ATOM   1110  CA  ASP A 152      26.034   5.514  34.649  1.00 30.85           C
ATOM   1111  C   ASP A 152      24.830   4.797  35.212  1.00 30.51           C
ATOM   1112  O   ASP A 152      24.779   3.562  35.137  1.00 30.29           O
ATOM   1113  CB  ASP A 152      27.178   4.965  35.519  1.00 31.48           C
ATOM   1114  CG  ASP A 152      28.384   5.812  35.493  1.00 34.64           C
ATOM   1115  OD1 ASP A 152      28.588   6.523  34.482  1.00 41.71           O
ATOM   1116  OD2 ASP A 152      29.177   5.857  36.437  1.00 37.31           O
ATOM   1117  N   THR A 153      23.894   5.501  35.833  1.00 30.21           N
ATOM   1118  CA  THR A 153      22.767   4.785  36.432  1.00 30.13           C
ATOM   1119  C   THR A 153      21.612   4.626  35.463  1.00 29.54           C
ATOM   1120  O   THR A 153      20.639   3.970  35.778  1.00 29.38           O
ATOM   1121  CB  THR A 153      22.277   5.481  37.704  1.00 30.37           C
ATOM   1122  OG1 THR A 153      21.735   6.770  37.373  1.00 31.06           O
ATOM   1123  CG2 THR A 153      23.452   5.763  38.658  1.00 30.56           C
ATOM   1124  N   VAL A 154      21.703   5.213  34.280  1.00 29.07           N
ATOM   1125  CA  VAL A 154      20.596   5.082  33.346  1.00 28.90           C
ATOM   1126  C   VAL A 154      20.488   3.613  32.968  1.00 28.83           C
ATOM   1127  O   VAL A 154      21.486   2.898  33.002  1.00 28.78           O
ATOM   1128  CB  VAL A 154      20.762   5.952  32.088  1.00 28.61           C
ATOM   1129  CG1 VAL A 154      20.808   7.410  32.462  1.00 29.14           C
ATOM   1130  CG2 VAL A 154      21.999   5.547  31.305  1.00 28.52           C
ATOM   1131  N   GLY A 155      19.283   3.170  32.615  1.00 28.74           N
ATOM   1132  CA  GLY A 155      19.043   1.780  32.263  1.00 28.33           C
ATOM   1133  C   GLY A 155      19.484   1.387  30.860  1.00 28.70           C
ATOM   1134  O   GLY A 155      19.862   2.235  30.031  1.00 28.27           O
ATOM   1135  N   ARG A 156      19.384   0.088  30.591  1.00 28.47           N
ATOM   1136  CA  ARG A 156      19.857  -0.519  29.349  1.00 28.54           C
ATOM   1137  C   ARG A 156      19.291   0.096  28.084  1.00 28.18           C
ATOM   1138  O   ARG A 156      20.029   0.346  27.143  1.00 28.69           O
ATOM   1139  CB  ARG A 156      19.582  -2.019  29.362  1.00 28.58           C
ATOM   1140  N   LYS A 157      17.986   0.304  28.042  1.00 27.53           N
ATOM   1141  CA  LYS A 157      17.390   0.888  26.860  1.00 27.32           C
ATOM   1142  C   LYS A 157      17.947   2.306  26.625  1.00 27.10           C
ATOM   1143  O   LYS A 157      18.213   2.672  25.490  1.00 26.76           O
ATOM   1144  CB  LYS A 157      15.858   0.902  26.960  1.00 27.68           C
ATOM   1145  CG  LYS A 157      15.171  -0.451  26.656  1.00 26.26           C
ATOM   1146  N   ILE A 158      18.138   3.086  27.688  1.00 26.68           N
ATOM   1147  CA  ILE A 158      18.665   4.450  27.543  1.00 26.67           C
ATOM   1148  C   ILE A 158      20.107   4.368  27.100  1.00 26.53           C
ATOM   1149  O   ILE A 158      20.558   5.170  26.285  1.00 25.74           O
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1150 | CB | ILE | A | 158 | 18.570 | 5.245 | 28.837 | 1.00 | 26.51 | C |
| ATOM | 1151 | CG1 | ILE | A | 158 | 17.114 | 5.399 | 29.269 | 1.00 | 27.11 | C |
| ATOM | 1152 | CG2 | ILE | A | 158 | 19.208 | 6.618 | 28.667 | 1.00 | 27.55 | C |
| ATOM | 1153 | CD1 | ILE | A | 158 | 16.232 | 6.028 | 28.260 | 1.00 | 28.98 | C |
| ATOM | 1154 | N | VAL | A | 159 | 20.817 | 3.378 | 27.629 | 1.00 | 26.46 | N |
| ATOM | 1155 | CA | VAL | A | 159 | 22.187 | 3.125 | 27.226 | 1.00 | 26.70 | C |
| ATOM | 1156 | C | VAL | A | 159 | 22.191 | 2.813 | 25.728 | 1.00 | 26.30 | C |
| ATOM | 1157 | O | VAL | A | 159 | 23.022 | 3.332 | 24.999 | 1.00 | 25.90 | O |
| ATOM | 1158 | CB | VAL | A | 159 | 22.819 | 1.963 | 28.018 | 1.00 | 27.18 | C |
| ATOM | 1159 | CG1 | VAL | A | 159 | 24.045 | 1.436 | 27.311 | 1.00 | 28.12 | C |
| ATOM | 1160 | CG2 | VAL | A | 159 | 23.180 | 2.410 | 29.427 | 1.00 | 27.44 | C |
| ATOM | 1161 | N | MET | A | 160 | 21.255 | 1.984 | 25.269 | 1.00 | 26.08 | N |
| ATOM | 1162 | CA | MET | A | 160 | 21.175 | 1.652 | 23.840 | 1.00 | 26.30 | C |
| ATOM | 1163 | C | MET | A | 160 | 20.906 | 2.929 | 23.005 | 1.00 | 24.71 | C |
| ATOM | 1164 | O | MET | A | 160 | 21.559 | 3.164 | 22.000 | 1.00 | 23.40 | O |
| ATOM | 1165 | CB | MET | A | 160 | 20.081 | 0.617 | 23.565 | 1.00 | 26.71 | C |
| ATOM | 1166 | CG | MET | A | 160 | 20.401 | -0.790 | 24.070 | 1.00 | 30.23 | C |
| ATOM | 1167 | SD | MET | A | 160 | 21.721 | -1.628 | 23.154 | 1.00 | 35.73 | S |
| ATOM | 1168 | CE | MET | A | 160 | 20.883 | -1.823 | 21.524 | 1.00 | 36.68 | C |
| ATOM | 1169 | N | ASP | A | 161 | 19.948 | 3.739 | 23.439 | 1.00 | 23.86 | N |
| ATOM | 1170 | CA | ASP | A | 161 | 19.636 | 5.000 | 22.756 | 1.00 | 23.67 | C |
| ATOM | 1171 | C | ASP | A | 161 | 20.840 | 5.943 | 22.664 | 1.00 | 22.65 | C |
| ATOM | 1172 | O | ASP | A | 161 | 21.148 | 6.478 | 21.593 | 1.00 | 23.02 | O |
| ATOM | 1173 | CB | ASP | A | 161 | 18.472 | 5.699 | 23.455 | 1.00 | 23.42 | C |
| ATOM | 1174 | CG | ASP | A | 161 | 17.178 | 4.898 | 23.369 | 1.00 | 24.19 | C |
| ATOM | 1175 | OD1 | ASP | A | 161 | 17.095 | 3.941 | 22.552 | 1.00 | 19.47 | O |
| ATOM | 1176 | OD2 | ASP | A | 161 | 16.197 | 5.164 | 24.087 | 1.00 | 24.90 | O |
| ATOM | 1177 | N | PHE | A | 162 | 21.513 | 6.132 | 23.791 | 1.00 | 21.70 | N |
| ATOM | 1178 | CA | PHE | A | 162 | 22.667 | 7.003 | 23.903 | 1.00 | 21.16 | C |
| ATOM | 1179 | C | PHE | A | 162 | 23.777 | 6.557 | 22.964 | 1.00 | 20.02 | C |
| ATOM | 1180 | O | PHE | A | 162 | 24.393 | 7.362 | 22.310 | 1.00 | 20.22 | O |
| ATOM | 1181 | CB | PHE | A | 162 | 23.144 | 7.010 | 25.364 | 1.00 | 21.38 | C |
| ATOM | 1182 | CG | PHE | A | 162 | 24.286 | 7.936 | 25.650 | 1.00 | 22.82 | C |
| ATOM | 1183 | CD1 | PHE | A | 162 | 24.072 | 9.290 | 25.882 | 1.00 | 26.05 | C |
| ATOM | 1184 | CD2 | PHE | A | 162 | 25.579 | 7.450 | 25.738 | 1.00 | 24.99 | C |
| ATOM | 1185 | CE1 | PHE | A | 162 | 25.144 | 10.136 | 26.181 | 1.00 | 25.32 | C |
| ATOM | 1186 | CE2 | PHE | A | 162 | 26.654 | 8.301 | 26.026 | 1.00 | 24.73 | C |
| ATOM | 1187 | CZ | PHE | A | 162 | 26.438 | 9.622 | 26.250 | 1.00 | 24.82 | C |
| ATOM | 1188 | N | LEU | A | 163 | 24.029 | 5.271 | 22.894 | 1.00 | 19.74 | N |
| ATOM | 1189 | CA | LEU | A | 163 | 25.064 | 4.767 | 21.998 | 1.00 | 19.88 | C |
| ATOM | 1190 | C | LEU | A | 163 | 24.688 | 4.965 | 20.533 | 1.00 | 18.90 | C |
| ATOM | 1191 | O | LEU | A | 163 | 25.554 | 5.020 | 19.675 | 1.00 | 18.20 | O |
| ATOM | 1192 | CB | LEU | A | 163 | 25.320 | 3.287 | 22.256 | 1.00 | 19.78 | C |
| ATOM | 1193 | CG | LEU | A | 163 | 26.078 | 3.019 | 23.546 | 1.00 | 20.79 | C |
| ATOM | 1194 | CD1 | LEU | A | 163 | 26.069 | 1.534 | 23.811 | 1.00 | 21.16 | C |
| ATOM | 1195 | CD2 | LEU | A | 163 | 27.498 | 3.567 | 23.456 | 1.00 | 21.66 | C |
| ATOM | 1196 | N | GLY | A | 164 | 23.395 | 5.055 | 20.272 | 1.00 | 18.33 | N |
| ATOM | 1197 | CA | GLY | A | 164 | 22.883 | 5.296 | 18.941 | 1.00 | 19.05 | C |
| ATOM | 1198 | C | GLY | A | 164 | 22.879 | 6.764 | 18.519 | 1.00 | 19.33 | C |
| ATOM | 1199 | O | GLY | A | 164 | 22.347 | 7.079 | 17.451 | 1.00 | 20.16 | O |
| ATOM | 1200 | N | PHE | A | 165 | 23.424 | 7.651 | 19.350 | 1.00 | 18.45 | N |
| ATOM | 1201 | CA | PHE | A | 165 | 23.516 | 9.048 | 18.974 | 1.00 | 19.26 | C |
| ATOM | 1202 | C | PHE | A | 165 | 24.548 | 9.102 | 17.850 | 1.00 | 19.34 | C |
| ATOM | 1203 | O | PHE | A | 165 | 25.363 | 8.177 | 17.720 | 1.00 | 18.77 | O |
| ATOM | 1204 | CB | PHE | A | 165 | 23.947 | 9.915 | 20.158 | 1.00 | 19.09 | C |
| ATOM | 1205 | CG | PHE | A | 165 | 22.862 | 10.139 | 21.208 | 1.00 | 20.44 | C |
| ATOM | 1206 | CD1 | PHE | A | 165 | 21.572 | 9.632 | 21.047 | 1.00 | 21.56 | C |
| ATOM | 1207 | CD2 | PHE | A | 165 | 23.143 | 10.878 | 22.357 | 1.00 | 20.27 | C |
| ATOM | 1208 | CE1 | PHE | A | 165 | 20.604 | 9.840 | 22.010 | 1.00 | 21.01 | C |
| ATOM | 1209 | CE2 | PHE | A | 165 | 22.174 | 11.096 | 23.326 | 1.00 | 20.14 | C |
| ATOM | 1210 | CZ | PHE | A | 165 | 20.913 | 10.567 | 23.163 | 1.00 | 22.00 | C |

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ATOM   1211  N   ASN A 166      24.508  10.157  17.040  1.00 19.48           N
ATOM   1212  CA  ASN A 166      25.428  10.290  15.897  1.00 20.08           C
ATOM   1213  C   ASN A 166      26.827  10.792  16.305  1.00 20.53           C
ATOM   1214  O   ASN A 166      27.193  11.975  16.076  1.00 20.34           O
ATOM   1215  CB  ASN A 166      24.836  11.183  14.790  1.00 19.52           C
ATOM   1216  CG  ASN A 166      25.572  11.003  13.451  1.00 19.82           C
ATOM   1217  OD1 ASN A 166      26.652  10.376  13.412  1.00 18.39           O
ATOM   1218  ND2 ASN A 166      24.987  11.528  12.350  1.00 15.25           N
ATOM   1219  N   TRP A 167      27.564   9.892  16.955  1.00 20.69           N
ATOM   1220  CA  TRP A 167      28.911  10.161  17.441  1.00 21.20           C
ATOM   1221  C   TRP A 167      29.858  10.404  16.270  1.00 21.35           C
ATOM   1222  O   TRP A 167      30.806  11.171  16.371  1.00 21.36           O
ATOM   1223  CB  TRP A 167      29.402   8.977  18.316  1.00 21.31           C
ATOM   1224  CG  TRP A 167      28.550   8.849  19.539  1.00 21.63           C
ATOM   1225  CD1 TRP A 167      27.673   7.841  19.844  1.00 22.35           C
ATOM   1226  CD2 TRP A 167      28.433   9.808  20.591  1.00 20.88           C
ATOM   1227  NE1 TRP A 167      27.030   8.119  21.028  1.00 22.98           N
ATOM   1228  CE2 TRP A 167      27.486   9.315  21.511  1.00 21.22           C
ATOM   1229  CE3 TRP A 167      29.054  11.036  20.863  1.00 20.14           C
ATOM   1230  CZ2 TRP A 167      27.143   9.999  22.670  1.00 22.17           C
ATOM   1231  CZ3 TRP A 167      28.693  11.724  21.990  1.00 19.81           C
ATOM   1232  CH2 TRP A 167      27.742  11.206  22.889  1.00 21.02           C
ATOM   1233  N   ASN A 168      29.610   9.743  15.153  1.00 21.50           N
ATOM   1234  CA  ASN A 168      30.464   9.927  13.991  1.00 21.77           C
ATOM   1235  C   ASN A 168      30.488  11.406  13.605  1.00 21.48           C
ATOM   1236  O   ASN A 168      31.549  11.992  13.428  1.00 20.55           O
ATOM   1237  CB  ASN A 168      29.964   9.101  12.814  1.00 22.00           C
ATOM   1238  CG  ASN A 168      30.856   9.236  11.584  1.00 23.99           C
ATOM   1239  OD1 ASN A 168      32.052   8.974  11.661  1.00 26.79           O
ATOM   1240  ND2 ASN A 168      30.277   9.652  10.448  1.00 24.40           N
ATOM   1241  N   TRP A 169      29.302  11.995  13.484  1.00 21.28           N
ATOM   1242  CA  TRP A 169      29.183  13.372  13.071  1.00 21.23           C
ATOM   1243  C   TRP A 169      29.708  14.331  14.133  1.00 21.44           C
ATOM   1244  O   TRP A 169      30.450  15.258  13.822  1.00 20.50           O
ATOM   1245  CB  TRP A 169      27.736  13.741  12.740  1.00 21.29           C
ATOM   1246  CG  TRP A 169      27.611  15.186  12.397  1.00 20.56           C
ATOM   1247  CD1 TRP A 169      27.840  15.766  11.173  1.00 19.81           C
ATOM   1248  CD2 TRP A 169      27.293  16.256  13.290  1.00 20.58           C
ATOM   1249  NE1 TRP A 169      27.641  17.124  11.253  1.00 20.45           N
ATOM   1250  CE2 TRP A 169      27.313  17.453  12.540  1.00 21.52           C
ATOM   1251  CE3 TRP A 169      26.951  16.324  14.636  1.00 22.34           C
ATOM   1252  CZ2 TRP A 169      27.036  18.705  13.102  1.00 24.24           C
ATOM   1253  CZ3 TRP A 169      26.690  17.558  15.195  1.00 24.93           C
ATOM   1254  CH2 TRP A 169      26.728  18.736  14.423  1.00 25.53           C
ATOM   1255  N   ILE A 170      29.318  14.124  15.381  1.00 21.81           N
ATOM   1256  CA  ILE A 170      29.742  15.056  16.412  1.00 22.51           C
ATOM   1257  C   ILE A 170      31.245  14.894  16.755  1.00 23.07           C
ATOM   1258  O   ILE A 170      31.917  15.872  17.067  1.00 23.88           O
ATOM   1259  CB  ILE A 170      28.837  14.988  17.662  1.00 21.97           C
ATOM   1260  CG1 ILE A 170      28.878  16.326  18.396  1.00 21.44           C
ATOM   1261  CG2 ILE A 170      29.262  13.894  18.581  1.00 21.76           C
ATOM   1262  CD1 ILE A 170      27.794  16.472  19.409  1.00 21.59           C
ATOM   1263  N   ASN A 171      31.781  13.692  16.674  1.00 23.52           N
ATOM   1264  CA  ASN A 171      33.209  13.516  16.934  1.00 24.55           C
ATOM   1265  C   ASN A 171      34.021  14.254  15.874  1.00 25.23           C
ATOM   1266  O   ASN A 171      35.067  14.828  16.171  1.00 25.14           O
ATOM   1267  CB  ASN A 171      33.626  12.031  16.949  1.00 24.52           C
ATOM   1268  CG  ASN A 171      33.095  11.271  18.171  1.00 24.45           C
ATOM   1269  OD1 ASN A 171      32.625  11.855  19.154  1.00 23.01           O
ATOM   1270  ND2 ASN A 171      33.169   9.969  18.099  1.00 22.49           N
ATOM   1271  N   LYS A 172      33.560  14.219  14.630  1.00 25.46           N
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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1272 | CA | LYS | A | 172 | 34.255 | 14.963 | 13.592 | 1.00 | 26.46 | C |
| ATOM | 1273 | C | LYS | A | 172 | 34.221 | 16.478 | 13.873 | 1.00 | 25.77 | C |
| ATOM | 1274 | O | LYS | A | 172 | 35.224 | 17.169 | 13.681 | 1.00 | 25.85 | O |
| ATOM | 1275 | CB | LYS | A | 172 | 33.705 | 14.634 | 12.205 | 1.00 | 26.90 | C |
| ATOM | 1276 | CG | LYS | A | 172 | 34.262 | 13.351 | 11.668 | 1.00 | 29.88 | C |
| ATOM | 1277 | CD | LYS | A | 172 | 33.752 | 13.033 | 10.240 | 1.00 | 34.20 | C |
| ATOM | 1278 | CE | LYS | A | 172 | 34.458 | 11.810 | 9.690 | 1.00 | 36.15 | C |
| ATOM | 1279 | NZ | LYS | A | 172 | 34.556 | 11.800 | 8.188 | 1.00 | 40.56 | N |
| ATOM | 1280 | N | GLN | A | 173 | 33.088 | 16.986 | 14.338 | 1.00 | 25.37 | N |
| ATOM | 1281 | CA | GLN | A | 173 | 32.981 | 18.400 | 14.690 | 1.00 | 25.52 | C |
| ATOM | 1282 | C | GLN | A | 173 | 34.002 | 18.741 | 15.774 | 1.00 | 25.71 | C |
| ATOM | 1283 | O | GLN | A | 173 | 34.780 | 19.669 | 15.618 | 1.00 | 26.05 | O |
| ATOM | 1284 | CB | GLN | A | 173 | 31.589 | 18.740 | 15.200 | 1.00 | 25.30 | C |
| ATOM | 1285 | CG | GLN | A | 173 | 30.522 | 18.729 | 14.138 | 1.00 | 25.28 | C |
| ATOM | 1286 | CD | GLN | A | 173 | 30.783 | 19.753 | 13.061 | 1.00 | 26.34 | C |
| ATOM | 1287 | OE1 | GLN | A | 173 | 31.252 | 20.872 | 13.345 | 1.00 | 26.57 | O |
| ATOM | 1288 | NE2 | GLN | A | 173 | 30.492 | 19.386 | 11.822 | 1.00 | 23.68 | N |
| ATOM | 1289 | N | GLN | A | 174 | 33.972 | 17.985 | 16.867 | 1.00 | 25.20 | N |
| ATOM | 1290 | CA | GLN | A | 174 | 34.931 | 18.124 | 17.944 | 1.00 | 25.45 | C |
| ATOM | 1291 | C | GLN | A | 174 | 36.380 | 18.182 | 17.392 | 1.00 | 25.74 | C |
| ATOM | 1292 | O | GLN | A | 174 | 37.152 | 19.066 | 17.767 | 1.00 | 24.76 | O |
| ATOM | 1293 | CB | GLN | A | 174 | 34.770 | 16.951 | 18.923 | 1.00 | 25.13 | C |
| ATOM | 1294 | CG | GLN | A | 174 | 35.771 | 16.925 | 20.048 | 1.00 | 26.00 | C |
| ATOM | 1295 | CD | GLN | A | 174 | 35.636 | 15.697 | 20.929 | 1.00 | 26.76 | C |
| ATOM | 1296 | OE1 | GLN | A | 174 | 35.278 | 14.629 | 20.450 | 1.00 | 28.02 | O |
| ATOM | 1297 | NE2 | GLN | A | 174 | 35.917 | 15.851 | 22.222 | 1.00 | 26.75 | N |
| ATOM | 1298 | N | GLY | A | 175 | 36.724 | 17.249 | 16.505 | 1.00 | 25.61 | N |
| ATOM | 1299 | CA | GLY | A | 175 | 38.040 | 17.201 | 15.887 | 1.00 | 26.56 | C |
| ATOM | 1300 | C | GLY | A | 175 | 38.333 | 18.393 | 14.980 | 1.00 | 27.62 | C |
| ATOM | 1301 | O | GLY | A | 175 | 39.371 | 19.051 | 15.111 | 1.00 | 28.21 | O |
| ATOM | 1302 | N | LYS | A | 176 | 37.415 | 18.695 | 14.074 | 1.00 | 28.41 | N |
| ATOM | 1303 | CA | LYS | A | 176 | 37.583 | 19.834 | 13.173 | 1.00 | 29.52 | C |
| ATOM | 1304 | C | LYS | A | 176 | 37.778 | 21.177 | 13.895 | 1.00 | 29.38 | C |
| ATOM | 1305 | O | LYS | A | 176 | 38.557 | 22.009 | 13.443 | 1.00 | 29.30 | O |
| ATOM | 1306 | CB | LYS | A | 176 | 36.371 | 19.977 | 12.257 | 1.00 | 29.90 | C |
| ATOM | 1307 | CG | LYS | A | 176 | 36.212 | 18.895 | 11.227 | 1.00 | 32.69 | C |
| ATOM | 1308 | CD | LYS | A | 176 | 35.023 | 19.242 | 10.336 | 1.00 | 36.10 | C |
| ATOM | 1309 | CE | LYS | A | 176 | 34.114 | 18.065 | 10.148 | 1.00 | 37.89 | C |
| ATOM | 1310 | NZ | LYS | A | 176 | 32.736 | 18.469 | 9.746 | 1.00 | 40.12 | N |
| ATOM | 1311 | N | ARG | A | 177 | 37.060 | 21.397 | 14.993 | 1.00 | 29.00 | N |
| ATOM | 1312 | CA | ARG | A | 177 | 37.164 | 22.671 | 15.710 | 1.00 | 29.17 | C |
| ATOM | 1313 | C | ARG | A | 177 | 38.260 | 22.741 | 16.781 | 1.00 | 28.13 | C |
| ATOM | 1314 | O | ARG | A | 177 | 38.433 | 23.788 | 17.394 | 1.00 | 27.46 | O |
| ATOM | 1315 | CB | ARG | A | 177 | 35.831 | 23.025 | 16.391 | 1.00 | 29.67 | C |
| ATOM | 1316 | CG | ARG | A | 177 | 34.606 | 22.876 | 15.536 | 1.00 | 31.86 | C |
| ATOM | 1317 | CD | ARG | A | 177 | 34.629 | 23.648 | 14.243 | 1.00 | 35.68 | C |
| ATOM | 1318 | NE | ARG | A | 177 | 33.691 | 23.034 | 13.313 | 1.00 | 38.08 | N |
| ATOM | 1319 | CZ | ARG | A | 177 | 33.865 | 22.938 | 12.015 | 1.00 | 40.57 | C |
| ATOM | 1320 | NH1 | ARG | A | 177 | 34.958 | 23.420 | 11.436 | 1.00 | 41.44 | N |
| ATOM | 1321 | NH2 | ARG | A | 177 | 32.927 | 22.362 | 11.283 | 1.00 | 42.98 | N |
| ATOM | 1322 | N | GLY | A | 178 | 38.972 | 21.640 | 17.014 | 1.00 | 27.36 | N |
| ATOM | 1323 | CA | GLY | A | 178 | 40.013 | 21.589 | 18.028 | 1.00 | 26.75 | C |
| ATOM | 1324 | C | GLY | A | 178 | 39.460 | 21.655 | 19.444 | 1.00 | 26.55 | C |
| ATOM | 1325 | O | GLY | A | 178 | 40.175 | 21.999 | 20.394 | 1.00 | 27.31 | O |
| ATOM | 1326 | N | TRP | A | 179 | 38.195 | 21.308 | 19.620 | 1.00 | 25.19 | N |
| ATOM | 1327 | CA | TRP | A | 179 | 37.626 | 21.379 | 20.947 | 1.00 | 25.17 | C |
| ATOM | 1328 | C | TRP | A | 179 | 38.257 | 20.404 | 21.926 | 1.00 | 25.28 | C |
| ATOM | 1329 | O | TRP | A | 179 | 38.909 | 19.454 | 21.541 | 1.00 | 24.67 | O |
| ATOM | 1330 | CB | TRP | A | 179 | 36.127 | 21.139 | 20.901 | 1.00 | 24.78 | C |
| ATOM | 1331 | CG | TRP | A | 179 | 35.364 | 22.197 | 20.201 | 1.00 | 24.55 | C |
| ATOM | 1332 | CD1 | TRP | A | 179 | 35.830 | 23.425 | 19.776 | 1.00 | 23.00 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1333 | CD2 | TRP | A | 179 | 33.985 | 22.140 | 19.825 | 1.00 | 24.35 | C |
| ATOM | 1334 | NE1 | TRP | A | 179 | 34.822 | 24.122 | 19.153 | 1.00 | 24.53 | N |
| ATOM | 1335 | CE2 | TRP | A | 179 | 33.676 | 23.355 | 19.167 | 1.00 | 24.34 | C |
| ATOM | 1336 | CE3 | TRP | A | 179 | 32.982 | 21.177 | 19.957 | 1.00 | 23.62 | C |
| ATOM | 1337 | CZ2 | TRP | A | 179 | 32.417 | 23.627 | 18.659 | 1.00 | 22.63 | C |
| ATOM | 1338 | CZ3 | TRP | A | 179 | 31.726 | 21.454 | 19.442 | 1.00 | 24.07 | C |
| ATOM | 1339 | CH2 | TRP | A | 179 | 31.453 | 22.674 | 18.811 | 1.00 | 23.17 | C |
| ATOM | 1340 | N | GLY | A | 180 | 38.061 | 20.669 | 23.210 | 1.00 | 25.61 | N |
| ATOM | 1341 | CA | GLY | A | 180 | 38.471 | 19.737 | 24.240 | 1.00 | 25.44 | C |
| ATOM | 1342 | C | GLY | A | 180 | 37.428 | 18.634 | 24.377 | 1.00 | 26.09 | C |
| ATOM | 1343 | O | GLY | A | 180 | 36.592 | 18.432 | 23.491 | 1.00 | 26.60 | O |
| ATOM | 1344 | N | GLN | A | 181 | 37.448 | 17.934 | 25.503 | 1.00 | 26.33 | N |
| ATOM | 1345 | CA | GLN | A | 181 | 36.561 | 16.806 | 25.708 | 1.00 | 26.77 | C |
| ATOM | 1346 | C | GLN | A | 181 | 35.099 | 17.180 | 25.953 | 1.00 | 26.26 | C |
| ATOM | 1347 | O | GLN | A | 181 | 34.775 | 18.291 | 26.371 | 1.00 | 25.90 | O |
| ATOM | 1348 | CB | GLN | A | 181 | 37.044 | 15.970 | 26.887 | 1.00 | 27.12 | C |
| ATOM | 1349 | CG | GLN | A | 181 | 36.689 | 16.543 | 28.269 | 1.00 | 29.66 | C |
| ATOM | 1350 | CD | GLN | A | 181 | 36.917 | 15.533 | 29.388 | 1.00 | 33.17 | C |
| ATOM | 1351 | OE1 | GLN | A | 181 | 38.055 | 15.295 | 29.791 | 1.00 | 35.52 | O |
| ATOM | 1352 | NE2 | GLN | A | 181 | 35.839 | 14.920 | 29.869 | 1.00 | 35.59 | N |
| ATOM | 1353 | N | LEU | A | 182 | 34.238 | 16.225 | 25.646 | 1.00 | 25.83 | N |
| ATOM | 1354 | CA | LEU | A | 182 | 32.831 | 16.241 | 26.021 | 1.00 | 25.59 | C |
| ATOM | 1355 | C | LEU | A | 182 | 32.850 | 16.162 | 27.543 | 1.00 | 24.45 | C |
| ATOM | 1356 | O | LEU | A | 182 | 33.433 | 15.209 | 28.084 | 1.00 | 23.27 | O |
| ATOM | 1357 | CB | LEU | A | 182 | 32.180 | 14.958 | 25.499 | 1.00 | 25.74 | C |
| ATOM | 1358 | CG | LEU | A | 182 | 30.666 | 14.790 | 25.403 | 1.00 | 28.29 | C |
| ATOM | 1359 | CD1 | LEU | A | 182 | 30.276 | 13.328 | 25.676 | 1.00 | 27.13 | C |
| ATOM | 1360 | CD2 | LEU | A | 182 | 29.928 | 15.671 | 26.303 | 1.00 | 30.64 | C |
| ATOM | 1361 | N | THR | A | 183 | 32.288 | 17.158 | 28.239 | 1.00 | 23.24 | N |
| ATOM | 1362 | CA | THR | A | 183 | 32.256 | 17.110 | 29.699 | 1.00 | 22.37 | C |
| ATOM | 1363 | C | THR | A | 183 | 30.956 | 16.504 | 30.150 | 1.00 | 22.01 | C |
| ATOM | 1364 | O | THR | A | 183 | 30.907 | 15.867 | 31.186 | 1.00 | 21.99 | O |
| ATOM | 1365 | CB | THR | A | 183 | 32.395 | 18.504 | 30.371 | 1.00 | 22.62 | C |
| ATOM | 1366 | OG1 | THR | A | 183 | 31.367 | 19.393 | 29.893 | 1.00 | 20.93 | O |
| ATOM | 1367 | CG2 | THR | A | 183 | 33.707 | 19.154 | 30.013 | 1.00 | 22.33 | C |
| ATOM | 1368 | N | SER | A | 184 | 29.885 | 16.711 | 29.396 | 1.00 | 21.54 | N |
| ATOM | 1369 | CA | SER | A | 184 | 28.622 | 16.146 | 29.810 | 1.00 | 21.58 | C |
| ATOM | 1370 | C | SER | A | 184 | 27.498 | 16.381 | 28.866 | 1.00 | 21.50 | C |
| ATOM | 1371 | O | SER | A | 184 | 27.610 | 17.168 | 27.928 | 1.00 | 21.85 | O |
| ATOM | 1372 | CB | SER | A | 184 | 28.209 | 16.715 | 31.158 | 1.00 | 21.78 | C |
| ATOM | 1373 | OG | SER | A | 184 | 27.856 | 18.072 | 31.056 | 1.00 | 23.20 | O |
| ATOM | 1374 | N | ASN | A | 185 | 26.416 | 15.667 | 29.134 | 1.00 | 21.14 | N |
| ATOM | 1375 | CA | ASN | A | 185 | 25.167 | 15.807 | 28.427 | 1.00 | 22.40 | C |
| ATOM | 1376 | C | ASN | A | 185 | 24.104 | 16.059 | 29.459 | 1.00 | 22.16 | C |
| ATOM | 1377 | O | ASN | A | 185 | 23.802 | 15.189 | 30.272 | 1.00 | 22.11 | O |
| ATOM | 1378 | CB | ASN | A | 185 | 24.794 | 14.523 | 27.664 | 1.00 | 22.46 | C |
| ATOM | 1379 | CG | ASN | A | 185 | 25.798 | 14.174 | 26.604 | 1.00 | 23.64 | C |
| ATOM | 1380 | OD1 | ASN | A | 185 | 26.582 | 13.257 | 26.789 | 1.00 | 25.26 | O |
| ATOM | 1381 | ND2 | ASN | A | 185 | 25.794 | 14.907 | 25.494 | 1.00 | 22.02 | N |
| ATOM | 1382 | N | LEU | A | 186 | 23.507 | 17.228 | 29.391 | 1.00 | 22.02 | N |
| ATOM | 1383 | CA | LEU | A | 186 | 22.461 | 17.600 | 30.319 | 1.00 | 22.34 | C |
| ATOM | 1384 | C | LEU | A | 186 | 21.114 | 17.251 | 29.707 | 1.00 | 22.21 | C |
| ATOM | 1385 | O | LEU | A | 186 | 20.808 | 17.623 | 28.582 | 1.00 | 22.59 | O |
| ATOM | 1386 | CB | LEU | A | 186 | 22.519 | 19.111 | 30.591 | 1.00 | 22.36 | C |
| ATOM | 1387 | CG | LEU | A | 186 | 21.650 | 19.642 | 31.739 | 1.00 | 23.03 | C |
| ATOM | 1388 | CD1 | LEU | A | 186 | 22.124 | 19.073 | 33.069 | 1.00 | 22.66 | C |
| ATOM | 1389 | CD2 | LEU | A | 186 | 21.636 | 21.213 | 31.782 | 1.00 | 21.88 | C |
| ATOM | 1390 | N | LEU | A | 187 | 20.307 | 16.530 | 30.461 | 1.00 | 22.39 | N |
| ATOM | 1391 | CA | LEU | A | 187 | 18.949 | 16.234 | 30.057 | 1.00 | 21.93 | C |
| ATOM | 1392 | C | LEU | A | 187 | 18.089 | 17.336 | 30.659 | 1.00 | 21.94 | C |
| ATOM | 1393 | O | LEU | A | 187 | 18.163 | 17.569 | 31.870 | 1.00 | 21.56 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1394 | CB | LEU | A | 187 | 18.525 | 14.883 | 30.604 | 1.00 | 21.36 | C |
| ATOM | 1395 | CG | LEU | A | 187 | 17.037 | 14.555 | 30.489 | 1.00 | 22.46 | C |
| ATOM | 1396 | CD1 | LEU | A | 187 | 16.550 | 14.530 | 29.038 | 1.00 | 22.25 | C |
| ATOM | 1397 | CD2 | LEU | A | 187 | 16.783 | 13.200 | 31.154 | 1.00 | 22.25 | C |
| ATOM | 1398 | N | LEU | A | 188 | 17.301 | 18.028 | 29.826 | 1.00 | 21.68 | N |
| ATOM | 1399 | CA | LEU | A | 188 | 16.400 | 19.052 | 30.329 | 1.00 | 22.46 | C |
| ATOM | 1400 | C | LEU | A | 188 | 14.925 | 18.743 | 30.021 | 1.00 | 22.70 | C |
| ATOM | 1401 | O | LEU | A | 188 | 14.511 | 18.622 | 28.864 | 1.00 | 23.01 | O |
| ATOM | 1402 | CB | LEU | A | 188 | 16.747 | 20.432 | 29.769 | 1.00 | 22.51 | C |
| ATOM | 1403 | CG | LEU | A | 188 | 18.166 | 20.932 | 29.998 | 1.00 | 24.09 | C |
| ATOM | 1404 | CD1 | LEU | A | 188 | 18.916 | 20.996 | 28.697 | 1.00 | 26.99 | C |
| ATOM | 1405 | CD2 | LEU | A | 188 | 18.135 | 22.308 | 30.564 | 1.00 | 25.94 | C |
| ATOM | 1406 | N | ILE | A | 189 | 14.117 | 18.652 | 31.061 | 1.00 | 22.31 | N |
| ATOM | 1407 | CA | ILE | A | 189 | 12.721 | 18.383 | 30.851 | 1.00 | 22.23 | C |
| ATOM | 1408 | C | ILE | A | 189 | 11.959 | 19.459 | 31.554 | 1.00 | 22.43 | C |
| ATOM | 1409 | O | ILE | A | 189 | 12.045 | 19.599 | 32.773 | 1.00 | 22.44 | O |
| ATOM | 1410 | CB | ILE | A | 189 | 12.328 | 17.009 | 31.369 | 1.00 | 21.56 | C |
| ATOM | 1411 | CG1 | ILE | A | 189 | 13.178 | 15.944 | 30.695 | 1.00 | 21.26 | C |
| ATOM | 1412 | CG2 | ILE | A | 189 | 10.873 | 16.794 | 31.078 | 1.00 | 21.74 | C |
| ATOM | 1413 | CD1 | ILE | A | 189 | 12.851 | 14.481 | 31.136 | 1.00 | 22.52 | C |
| ATOM | 1414 | N | GLY | A | 190 | 11.226 | 20.239 | 30.770 | 1.00 | 23.11 | N |
| ATOM | 1415 | CA | GLY | A | 190 | 10.545 | 21.396 | 31.294 | 1.00 | 23.06 | C |
| ATOM | 1416 | C | GLY | A | 190 | 9.084 | 21.395 | 30.988 | 1.00 | 23.56 | C |
| ATOM | 1417 | O | GLY | A | 190 | 8.594 | 20.646 | 30.117 | 1.00 | 23.29 | O |
| ATOM | 1418 | N | MET | A | 191 | 8.385 | 22.224 | 31.755 | 1.00 | 24.04 | N |
| ATOM | 1419 | CA | MET | A | 191 | 6.980 | 22.468 | 31.542 | 1.00 | 24.73 | C |
| ATOM | 1420 | C | MET | A | 191 | 6.837 | 23.623 | 30.576 | 1.00 | 24.58 | C |
| ATOM | 1421 | O | MET | A | 191 | 7.747 | 24.464 | 30.443 | 1.00 | 24.72 | O |
| ATOM | 1422 | CB | MET | A | 191 | 6.301 | 22.821 | 32.860 | 1.00 | 25.52 | C |
| ATOM | 1423 | CG | MET | A | 191 | 6.212 | 21.649 | 33.806 | 1.00 | 26.99 | C |
| ATOM | 1424 | SD | MET | A | 191 | 5.710 | 22.122 | 35.447 | 1.00 | 30.62 | S |
| ATOM | 1425 | CE | MET | A | 191 | 4.076 | 22.639 | 35.135 | 1.00 | 32.05 | C |
| ATOM | 1426 | N | GLU | A | 192 | 5.701 | 23.659 | 29.893 | 1.00 | 24.37 | N |
| ATOM | 1427 | CA | GLU | A | 192 | 5.407 | 24.718 | 28.940 | 1.00 | 24.51 | C |
| ATOM | 1428 | C | GLU | A | 192 | 5.468 | 26.072 | 29.628 | 1.00 | 24.20 | C |
| ATOM | 1429 | O | GLU | A | 192 | 5.013 | 26.237 | 30.745 | 1.00 | 24.12 | O |
| ATOM | 1430 | CB | GLU | A | 192 | 4.029 | 24.514 | 28.342 | 1.00 | 24.59 | C |
| ATOM | 1431 | CG | GLU | A | 192 | 2.930 | 24.487 | 29.384 | 1.00 | 26.08 | C |
| ATOM | 1432 | CD | GLU | A | 192 | 1.590 | 24.051 | 28.830 | 1.00 | 26.38 | C |
| ATOM | 1433 | OE1 | GLU | A | 192 | 1.530 | 23.568 | 27.676 | 1.00 | 27.04 | O |
| ATOM | 1434 | OE2 | GLU | A | 192 | 0.599 | 24.219 | 29.562 | 1.00 | 25.46 | O |
| ATOM | 1435 | N | GLY | A | 193 | 6.045 | 27.051 | 28.962 | 1.00 | 24.44 | N |
| ATOM | 1436 | CA | GLY | A | 193 | 6.153 | 28.364 | 29.562 | 1.00 | 24.21 | C |
| ATOM | 1437 | C | GLY | A | 193 | 7.428 | 28.565 | 30.358 | 1.00 | 23.71 | C |
| ATOM | 1438 | O | GLY | A | 193 | 7.728 | 29.691 | 30.697 | 1.00 | 24.97 | O |
| ATOM | 1439 | N | ASN | A | 194 | 8.181 | 27.507 | 30.663 | 1.00 | 23.27 | N |
| ATOM | 1440 | CA | ASN | A | 194 | 9.445 | 27.656 | 31.413 | 1.00 | 22.47 | C |
| ATOM | 1441 | C | ASN | A | 194 | 10.465 | 28.476 | 30.636 | 1.00 | 22.35 | C |
| ATOM | 1442 | O | ASN | A | 194 | 10.594 | 28.317 | 29.416 | 1.00 | 22.38 | O |
| ATOM | 1443 | CB | ASN | A | 194 | 10.108 | 26.299 | 31.708 | 1.00 | 22.17 | C |
| ATOM | 1444 | CG | ASN | A | 194 | 9.476 | 25.555 | 32.882 | 1.00 | 22.24 | C |
| ATOM | 1445 | OD1 | ASN | A | 194 | 8.477 | 25.992 | 33.453 | 1.00 | 23.81 | O |
| ATOM | 1446 | ND2 | ASN | A | 194 | 10.075 | 24.429 | 33.253 | 1.00 | 18.58 | N |
| ATOM | 1447 | N | VAL | A | 195 | 11.226 | 29.295 | 31.362 | 1.00 | 21.64 | N |
| ATOM | 1448 | CA | VAL | A | 195 | 12.263 | 30.114 | 30.789 | 1.00 | 21.41 | C |
| ATOM | 1449 | C | VAL | A | 195 | 13.569 | 29.988 | 31.556 | 1.00 | 20.40 | C |
| ATOM | 1450 | O | VAL | A | 195 | 13.603 | 30.014 | 32.790 | 1.00 | 20.03 | O |
| ATOM | 1451 | CB | VAL | A | 195 | 11.889 | 31.621 | 30.828 | 1.00 | 21.72 | C |
| ATOM | 1452 | CG1 | VAL | A | 195 | 13.038 | 32.476 | 30.327 | 1.00 | 21.84 | C |
| ATOM | 1453 | CG2 | VAL | A | 195 | 10.628 | 31.904 | 30.043 | 1.00 | 23.61 | C |
| ATOM | 1454 | N | THR | A | 196 | 14.644 | 29.834 | 30.813 | 1.00 | 19.77 | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1455 | CA | THR | A | 196 | 15.980 | 29.917 | 31.376 | 1.00 | 20.37 | C |
| ATOM | 1456 | C | THR | A | 196 | 16.467 | 31.291 | 30.933 | 1.00 | 20.92 | C |
| ATOM | 1457 | O | THR | A | 196 | 16.649 | 31.505 | 29.724 | 1.00 | 20.45 | O |
| ATOM | 1458 | CB | THR | A | 196 | 16.882 | 28.865 | 30.793 | 1.00 | 19.87 | C |
| ATOM | 1459 | OG1 | THR | A | 196 | 16.457 | 27.564 | 31.227 | 1.00 | 21.07 | O |
| ATOM | 1460 | CG2 | THR | A | 196 | 18.273 | 29.043 | 31.340 | 1.00 | 20.00 | C |
| ATOM | 1461 | N | PRO | A | 197 | 16.602 | 32.225 | 31.879 | 1.00 | 21.53 | N |
| ATOM | 1462 | CA | PRO | A | 197 | 16.997 | 33.609 | 31.572 | 1.00 | 22.24 | C |
| ATOM | 1463 | C | PRO | A | 197 | 18.375 | 33.688 | 30.952 | 1.00 | 22.26 | C |
| ATOM | 1464 | O | PRO | A | 197 | 19.195 | 32.773 | 31.130 | 1.00 | 22.66 | O |
| ATOM | 1465 | CB | PRO | A | 197 | 16.998 | 34.305 | 32.934 | 1.00 | 22.51 | C |
| ATOM | 1466 | CG | PRO | A | 197 | 16.282 | 33.411 | 33.839 | 1.00 | 22.92 | C |
| ATOM | 1467 | CD | PRO | A | 197 | 16.367 | 32.028 | 33.312 | 1.00 | 21.85 | C |
| ATOM | 1468 | N | ALA | A | 198 | 18.606 | 34.776 | 30.234 | 1.00 | 21.54 | N |
| ATOM | 1469 | CA | ALA | A | 198 | 19.821 | 34.976 | 29.486 | 1.00 | 21.47 | C |
| ATOM | 1470 | C | ALA | A | 198 | 21.110 | 34.764 | 30.282 | 1.00 | 21.22 | C |
| ATOM | 1471 | O | ALA | A | 198 | 21.298 | 35.310 | 31.386 | 1.00 | 20.56 | O |
| ATOM | 1472 | CB | ALA | A | 198 | 19.809 | 36.397 | 28.891 | 1.00 | 21.92 | C |
| ATOM | 1473 | N | HIS | A | 199 | 22.023 | 34.020 | 29.683 | 1.00 | 21.01 | N |
| ATOM | 1474 | CA | HIS | A | 199 | 23.321 | 33.764 | 30.288 | 1.00 | 21.40 | C |
| ATOM | 1475 | C | HIS | A | 199 | 24.250 | 33.279 | 29.213 | 1.00 | 21.61 | C |
| ATOM | 1476 | O | HIS | A | 199 | 23.811 | 33.017 | 28.089 | 1.00 | 21.18 | O |
| ATOM | 1477 | CB | HIS | A | 199 | 23.217 | 32.669 | 31.338 | 1.00 | 21.05 | C |
| ATOM | 1478 | CG | HIS | A | 199 | 22.864 | 31.354 | 30.746 | 1.00 | 22.98 | C |
| ATOM | 1479 | ND1 | HIS | A | 199 | 21.576 | 31.048 | 30.370 | 1.00 | 21.97 | N |
| ATOM | 1480 | CD2 | HIS | A | 199 | 23.630 | 30.287 | 30.399 | 1.00 | 21.48 | C |
| ATOM | 1481 | CE1 | HIS | A | 199 | 21.558 | 29.838 | 29.838 | 1.00 | 22.85 | C |
| ATOM | 1482 | NE2 | HIS | A | 199 | 22.791 | 29.368 | 29.821 | 1.00 | 24.36 | N |
| ATOM | 1483 | N | TYR | A | 200 | 25.538 | 33.177 | 29.555 | 1.00 | 22.22 | N |
| ATOM | 1484 | CA | TYR | A | 200 | 26.531 | 32.597 | 28.654 | 1.00 | 22.56 | C |
| ATOM | 1485 | C | TYR | A | 200 | 27.234 | 31.448 | 29.380 | 1.00 | 22.96 | C |
| ATOM | 1486 | O | TYR | A | 200 | 27.293 | 31.430 | 30.612 | 1.00 | 22.90 | O |
| ATOM | 1487 | CB | TYR | A | 200 | 27.528 | 33.610 | 28.129 | 1.00 | 22.56 | C |
| ATOM | 1488 | CG | TYR | A | 200 | 28.492 | 34.228 | 29.145 | 1.00 | 23.02 | C |
| ATOM | 1489 | CD1 | TYR | A | 200 | 29.731 | 33.671 | 29.385 | 1.00 | 22.79 | C |
| ATOM | 1490 | CD2 | TYR | A | 200 | 28.180 | 35.419 | 29.799 | 1.00 | 23.89 | C |
| ATOM | 1491 | CE1 | TYR | A | 200 | 30.612 | 34.229 | 30.283 | 1.00 | 22.32 | C |
| ATOM | 1492 | CE2 | TYR | A | 200 | 29.062 | 35.991 | 30.722 | 1.00 | 22.06 | C |
| ATOM | 1493 | CZ | TYR | A | 200 | 30.277 | 35.402 | 30.947 | 1.00 | 22.13 | C |
| ATOM | 1494 | OH | TYR | A | 200 | 31.163 | 35.957 | 31.843 | 1.00 | 20.46 | O |
| ATOM | 1495 | N | ASP | A | 201 | 27.723 | 30.467 | 28.619 | 1.00 | 23.11 | N |
| ATOM | 1496 | CA | ASP | A | 201 | 28.433 | 29.326 | 29.213 | 1.00 | 23.02 | C |
| ATOM | 1497 | C | ASP | A | 201 | 29.833 | 29.338 | 28.687 | 1.00 | 23.38 | C |
| ATOM | 1498 | O | ASP | A | 201 | 30.038 | 29.811 | 27.597 | 1.00 | 24.05 | O |
| ATOM | 1499 | CB | ASP | A | 201 | 27.776 | 28.012 | 28.829 | 1.00 | 22.85 | C |
| ATOM | 1500 | CG | ASP | A | 201 | 26.365 | 27.898 | 29.338 | 1.00 | 21.12 | C |
| ATOM | 1501 | OD1 | ASP | A | 201 | 26.176 | 27.802 | 30.568 | 1.00 | 23.22 | O |
| ATOM | 1502 | OD2 | ASP | A | 201 | 25.387 | 27.845 | 28.574 | 1.00 | 20.55 | O |
| ATOM | 1503 | N | GLU | A | 202 | 30.799 | 28.820 | 29.437 | 1.00 | 23.78 | N |
| ATOM | 1504 | CA | GLU | A | 202 | 32.184 | 28.782 | 28.950 | 1.00 | 25.14 | C |
| ATOM | 1505 | C | GLU | A | 202 | 32.524 | 27.467 | 28.269 | 1.00 | 24.96 | C |
| ATOM | 1506 | O | GLU | A | 202 | 33.657 | 27.001 | 28.394 | 1.00 | 26.76 | O |
| ATOM | 1507 | CB | GLU | A | 202 | 33.218 | 28.965 | 30.091 | 1.00 | 24.67 | C |
| ATOM | 1508 | CG | GLU | A | 202 | 33.017 | 30.199 | 30.941 | 1.00 | 27.79 | C |
| ATOM | 1509 | CD | GLU | A | 202 | 34.089 | 30.312 | 32.025 | 1.00 | 30.13 | C |
| ATOM | 1510 | OE1 | GLU | A | 202 | 34.018 | 29.584 | 33.030 | 1.00 | 32.67 | O |
| ATOM | 1511 | OE2 | GLU | A | 202 | 35.010 | 31.114 | 31.844 | 1.00 | 29.05 | O |
| ATOM | 1512 | N | GLN | A | 203 | 31.547 | 26.818 | 27.653 | 1.00 | 24.30 | N |
| ATOM | 1513 | CA | GLN | A | 203 | 31.804 | 25.624 | 26.874 | 1.00 | 23.24 | C |
| ATOM | 1514 | C | GLN | A | 203 | 31.036 | 25.764 | 25.572 | 1.00 | 22.84 | C |
| ATOM | 1515 | O | GLN | A | 203 | 30.122 | 26.560 | 25.468 | 1.00 | 23.00 | O |

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ATOM   1516  CB  GLN A 203      31.373  24.363  27.618  1.00 23.43           C
ATOM   1517  CG  GLN A 203      32.256  24.031  28.826  1.00 23.66           C
ATOM   1518  CD  GLN A 203      32.061  22.612  29.354  1.00 25.58           C
ATOM   1519  OE1 GLN A 203      31.915  21.661  28.582  1.00 27.85           O
ATOM   1520  NE2 GLN A 203      32.084  22.468  30.670  1.00 25.67           N
ATOM   1521  N   GLN A 204      31.465  25.013  24.575  1.00 22.51           N
ATOM   1522  CA  GLN A 204      30.791  24.910  23.299  1.00 22.51           C
ATOM   1523  C   GLN A 204      29.626  23.980  23.504  1.00 21.70           C
ATOM   1524  O   GLN A 204      29.737  23.026  24.255  1.00 21.24           O
ATOM   1525  CB  GLN A 204      31.718  24.307  22.255  1.00 22.29           C
ATOM   1526  CG  GLN A 204      33.001  25.081  22.072  1.00 22.69           C
ATOM   1527  CD  GLN A 204      32.820  26.346  21.259  1.00 22.39           C
ATOM   1528  OE1 GLN A 204      31.699  26.736  20.932  1.00 19.22           O
ATOM   1529  NE2 GLN A 204      33.937  26.970  20.906  1.00 19.77           N
ATOM   1530  N   ASN A 205      28.523  24.241  22.810  1.00 21.48           N
ATOM   1531  CA  ASN A 205      27.309  23.471  23.017  1.00 21.04           C
ATOM   1532  C   ASN A 205      26.558  23.136  21.730  1.00 21.10           C
ATOM   1533  O   ASN A 205      26.188  24.043  20.949  1.00 20.02           O
ATOM   1534  CB  ASN A 205      26.401  24.322  23.920  1.00 21.70           C
ATOM   1535  CG  ASN A 205      25.084  23.654  24.269  1.00 21.87           C
ATOM   1536  OD1 ASN A 205      24.732  22.577  23.775  1.00 22.07           O
ATOM   1537  ND2 ASN A 205      24.332  24.320  25.118  1.00 19.37           N
ATOM   1538  N   PHE A 206      26.350  21.835  21.497  1.00 20.28           N
ATOM   1539  CA  PHE A 206      25.372  21.414  20.523  1.00 20.14           C
ATOM   1540  C   PHE A 206      24.141  21.030  21.323  1.00 19.94           C
ATOM   1541  O   PHE A 206      24.164  20.052  22.065  1.00 20.71           O
ATOM   1542  CB  PHE A 206      25.851  20.238  19.693  1.00 20.65           C
ATOM   1543  CG  PHE A 206      26.799  20.618  18.620  1.00 20.30           C
ATOM   1544  CD1 PHE A 206      26.394  21.438  17.600  1.00 20.89           C
ATOM   1545  CD2 PHE A 206      28.101  20.168  18.642  1.00 21.26           C
ATOM   1546  CE1 PHE A 206      27.254  21.783  16.605  1.00 22.17           C
ATOM   1547  CE2 PHE A 206      28.980  20.523  17.641  1.00 21.31           C
ATOM   1548  CZ  PHE A 206      28.558  21.336  16.632  1.00 21.79           C
ATOM   1549  N   PHE A 207      23.058  21.764  21.081  1.00 19.87           N
ATOM   1550  CA  PHE A 207      21.790  21.723  21.824  1.00 20.08           C
ATOM   1551  C   PHE A 207      20.766  20.988  20.975  1.00 20.29           C
ATOM   1552  O   PHE A 207      20.276  21.519  20.011  1.00 19.94           O
ATOM   1553  CB  PHE A 207      21.385  23.190  22.083  1.00 20.46           C
ATOM   1554  CG  PHE A 207      20.129  23.404  22.890  1.00 19.14           C
ATOM   1555  CD1 PHE A 207      18.947  23.708  22.267  1.00 19.77           C
ATOM   1556  CD2 PHE A 207      20.169  23.428  24.259  1.00 19.99           C
ATOM   1557  CE1 PHE A 207      17.818  23.980  22.984  1.00 21.67           C
ATOM   1558  CE2 PHE A 207      19.037  23.683  24.992  1.00 22.36           C
ATOM   1559  CZ  PHE A 207      17.854  23.975  24.351  1.00 22.30           C
ATOM   1560  N   ALA A 208      20.480  19.746  21.352  1.00 21.01           N
ATOM   1561  CA  ALA A 208      19.688  18.827  20.541  1.00 21.26           C
ATOM   1562  C   ALA A 208      18.260  18.669  21.030  1.00 21.74           C
ATOM   1563  O   ALA A 208      18.000  17.983  22.049  1.00 21.21           O
ATOM   1564  CB  ALA A 208      20.365  17.464  20.557  1.00 20.94           C
ATOM   1565  N   GLN A 209      17.329  19.245  20.276  1.00 21.56           N
ATOM   1566  CA  GLN A 209      15.940  19.219  20.697  1.00 21.78           C
ATOM   1567  C   GLN A 209      15.289  17.864  20.393  1.00 21.84           C
ATOM   1568  O   GLN A 209      15.506  17.245  19.323  1.00 20.40           O
ATOM   1569  CB  GLN A 209      15.203  20.391  20.068  1.00 22.08           C
ATOM   1570  CG  GLN A 209      13.790  20.597  20.542  1.00 22.02           C
ATOM   1571  CD  GLN A 209      13.688  20.986  22.013  1.00 22.84           C
ATOM   1572  OE1 GLN A 209      14.700  21.240  22.678  1.00 22.55           O
ATOM   1573  NE2 GLN A 209      12.448  21.034  22.524  1.00 21.97           N
ATOM   1574  N   ILE A 210      14.480  17.418  21.351  1.00 22.17           N
ATOM   1575  CA  ILE A 210      13.904  16.084  21.329  1.00 22.53           C
ATOM   1576  C   ILE A 210      12.397  16.074  21.316  1.00 23.45           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1577 | O | ILE | A | 210 | 11.813 | 15.429 | 20.467 | 1.00 | 24.08 | O |
| ATOM | 1578 | CB | ILE | A | 210 | 14.411 | 15.306 | 22.541 | 1.00 | 22.81 | C |
| ATOM | 1579 | CG1 | ILE | A | 210 | 15.857 | 14.886 | 22.284 | 1.00 | 23.77 | C |
| ATOM | 1580 | CG2 | ILE | A | 210 | 13.573 | 14.064 | 22.785 | 1.00 | 23.17 | C |
| ATOM | 1581 | CD1 | ILE | A | 210 | 16.631 | 14.512 | 23.519 | 1.00 | 24.86 | C |
| ATOM | 1582 | N | LYS | A | 211 | 11.772 | 16.778 | 22.258 | 1.00 | 23.73 | N |
| ATOM | 1583 | CA | LYS | A | 211 | 10.318 | 16.829 | 22.351 | 1.00 | 22.99 | C |
| ATOM | 1584 | C | LYS | A | 211 | 9.873 | 18.253 | 22.566 | 1.00 | 22.73 | C |
| ATOM | 1585 | O | LYS | A | 211 | 10.436 | 18.969 | 23.391 | 1.00 | 22.34 | O |
| ATOM | 1586 | CB | LYS | A | 211 | 9.818 | 16.014 | 23.527 | 1.00 | 23.40 | C |
| ATOM | 1587 | CG | LYS | A | 211 | 8.285 | 15.757 | 23.509 | 1.00 | 24.55 | C |
| ATOM | 1588 | CD | LYS | A | 211 | 7.794 | 15.232 | 24.870 | 1.00 | 25.75 | C |
| ATOM | 1589 | CE | LYS | A | 211 | 6.389 | 14.579 | 24.861 | 1.00 | 25.61 | C |
| ATOM | 1590 | NZ | LYS | A | 211 | 5.580 | 14.641 | 23.613 | 1.00 | 25.29 | N |
| ATOM | 1591 | N | GLY | A | 212 | 8.832 | 18.655 | 21.847 | 1.00 | 22.34 | N |
| ATOM | 1592 | CA | GLY | A | 212 | 8.292 | 19.989 | 21.983 | 1.00 | 22.46 | C |
| ATOM | 1593 | C | GLY | A | 212 | 9.188 | 21.026 | 21.338 | 1.00 | 22.40 | C |
| ATOM | 1594 | O | GLY | A | 212 | 10.172 | 20.705 | 20.650 | 1.00 | 21.93 | O |
| ATOM | 1595 | N | TYR | A | 213 | 8.859 | 22.281 | 21.592 | 1.00 | 22.95 | N |
| ATOM | 1596 | CA | TYR | A | 213 | 9.530 | 23.400 | 20.944 | 1.00 | 23.32 | C |
| ATOM | 1597 | C | TYR | A | 213 | 10.079 | 24.412 | 21.926 | 1.00 | 23.27 | C |
| ATOM | 1598 | O | TYR | A | 213 | 9.434 | 24.740 | 22.918 | 1.00 | 23.34 | O |
| ATOM | 1599 | CB | TYR | A | 213 | 8.547 | 24.092 | 20.012 | 1.00 | 23.77 | C |
| ATOM | 1600 | CG | TYR | A | 213 | 8.133 | 23.198 | 18.887 | 1.00 | 25.58 | C |
| ATOM | 1601 | CD1 | TYR | A | 213 | 7.110 | 22.261 | 19.041 | 1.00 | 28.74 | C |
| ATOM | 1602 | CD2 | TYR | A | 213 | 8.798 | 23.253 | 17.687 | 1.00 | 28.55 | C |
| ATOM | 1603 | CE1 | TYR | A | 213 | 6.764 | 21.410 | 17.995 | 1.00 | 30.77 | C |
| ATOM | 1604 | CE2 | TYR | A | 213 | 8.465 | 22.429 | 16.651 | 1.00 | 30.41 | C |
| ATOM | 1605 | CZ | TYR | A | 213 | 7.461 | 21.516 | 16.795 | 1.00 | 31.44 | C |
| ATOM | 1606 | OH | TYR | A | 213 | 7.188 | 20.720 | 15.708 | 1.00 | 35.50 | O |
| ATOM | 1607 | N | LYS | A | 214 | 11.270 | 24.911 | 21.620 | 1.00 | 22.60 | N |
| ATOM | 1608 | CA | LYS | A | 214 | 11.916 | 25.911 | 22.431 | 1.00 | 22.58 | C |
| ATOM | 1609 | C | LYS | A | 214 | 12.353 | 27.077 | 21.576 | 1.00 | 22.52 | C |
| ATOM | 1610 | O | LYS | A | 214 | 12.937 | 26.898 | 20.493 | 1.00 | 23.74 | O |
| ATOM | 1611 | CB | LYS | A | 214 | 13.132 | 25.345 | 23.169 | 1.00 | 22.31 | C |
| ATOM | 1612 | CG | LYS | A | 214 | 12.784 | 24.539 | 24.392 | 1.00 | 22.79 | C |
| ATOM | 1613 | CD | LYS | A | 214 | 14.053 | 24.007 | 25.077 | 1.00 | 22.96 | C |
| ATOM | 1614 | CE | LYS | A | 214 | 13.821 | 23.675 | 26.530 | 1.00 | 20.69 | C |
| ATOM | 1615 | NZ | LYS | A | 214 | 15.076 | 23.085 | 27.149 | 1.00 | 19.14 | N |
| ATOM | 1616 | N | ARG | A | 215 | 12.037 | 28.277 | 22.047 | 1.00 | 21.95 | N |
| ATOM | 1617 | CA | ARG | A | 215 | 12.480 | 29.482 | 21.378 | 1.00 | 21.48 | C |
| ATOM | 1618 | C | ARG | A | 215 | 13.790 | 29.864 | 22.018 | 1.00 | 21.06 | C |
| ATOM | 1619 | O | ARG | A | 215 | 13.890 | 29.954 | 23.230 | 1.00 | 20.53 | O |
| ATOM | 1620 | CB | ARG | A | 215 | 11.466 | 30.582 | 21.576 | 1.00 | 22.15 | C |
| ATOM | 1621 | CG | ARG | A | 215 | 11.843 | 31.913 | 20.969 | 1.00 | 22.00 | C |
| ATOM | 1622 | CD | ARG | A | 215 | 11.231 | 33.041 | 21.727 | 1.00 | 23.87 | C |
| ATOM | 1623 | NE | ARG | A | 215 | 11.224 | 34.272 | 20.959 | 1.00 | 25.87 | N |
| ATOM | 1624 | CZ | ARG | A | 215 | 10.566 | 35.364 | 21.297 | 1.00 | 25.54 | C |
| ATOM | 1625 | NH1 | ARG | A | 215 | 9.873 | 35.425 | 22.423 | 1.00 | 24.05 | N |
| ATOM | 1626 | NH2 | ARG | A | 215 | 10.634 | 36.420 | 20.505 | 1.00 | 29.37 | N |
| ATOM | 1627 | N | CYS | A | 216 | 14.794 | 30.090 | 21.193 | 1.00 | 21.48 | N |
| ATOM | 1628 | CA | CYS | A | 216 | 16.123 | 30.355 | 21.668 | 1.00 | 21.40 | C |
| ATOM | 1629 | C | CYS | A | 216 | 16.533 | 31.723 | 21.146 | 1.00 | 21.86 | C |
| ATOM | 1630 | O | CYS | A | 216 | 16.532 | 31.952 | 19.948 | 1.00 | 22.82 | O |
| ATOM | 1631 | CB | CYS | A | 216 | 17.079 | 29.309 | 21.127 | 1.00 | 21.46 | C |
| ATOM | 1632 | SG | CYS | A | 216 | 16.689 | 27.562 | 21.469 | 1.00 | 22.63 | S |
| ATOM | 1633 | N | ILE | A | 217 | 16.878 | 32.630 | 22.045 | 1.00 | 21.29 | N |
| ATOM | 1634 | CA | ILE | A | 217 | 17.331 | 33.960 | 21.663 | 1.00 | 21.28 | C |
| ATOM | 1635 | C | ILE | A | 217 | 18.782 | 34.114 | 22.102 | 1.00 | 20.86 | C |
| ATOM | 1636 | O | ILE | A | 217 | 19.085 | 34.007 | 23.310 | 1.00 | 21.04 | O |
| ATOM | 1637 | CB | ILE | A | 217 | 16.456 | 35.025 | 22.327 | 1.00 | 21.80 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1638 | CG1 | ILE | A | 217 | 14.978 | 34.807 | 21.955 | 1.00 | 22.90 | C |
| ATOM | 1639 | CG2 | ILE | A | 217 | 16.874 | 36.414 | 21.861 | 1.00 | 22.72 | C |
| ATOM | 1640 | CD1 | ILE | A | 217 | 14.031 | 35.695 | 22.693 | 1.00 | 24.99 | C |
| ATOM | 1641 | N | LEU | A | 218 | 19.666 | 34.346 | 21.128 | 1.00 | 20.25 | N |
| ATOM | 1642 | CA | LEU | A | 218 | 21.094 | 34.451 | 21.373 | 1.00 | 20.55 | C |
| ATOM | 1643 | C | LEU | A | 218 | 21.630 | 35.853 | 21.128 | 1.00 | 21.19 | C |
| ATOM | 1644 | O | LEU | A | 218 | 21.141 | 36.560 | 20.253 | 1.00 | 21.62 | O |
| ATOM | 1645 | CB | LEU | A | 218 | 21.874 | 33.493 | 20.467 | 1.00 | 20.31 | C |
| ATOM | 1646 | CG | LEU | A | 218 | 21.964 | 32.019 | 20.906 | 1.00 | 20.46 | C |
| ATOM | 1647 | CD1 | LEU | A | 218 | 20.628 | 31.415 | 21.054 | 1.00 | 20.19 | C |
| ATOM | 1648 | CD2 | LEU | A | 218 | 22.732 | 31.229 | 19.907 | 1.00 | 22.84 | C |
| ATOM | 1649 | N | PHE | A | 219 | 22.658 | 36.231 | 21.886 | 1.00 | 21.06 | N |
| ATOM | 1650 | CA | PHE | A | 219 | 23.331 | 37.498 | 21.682 | 1.00 | 21.62 | C |
| ATOM | 1651 | C | PHE | A | 219 | 24.842 | 37.244 | 21.611 | 1.00 | 21.87 | C |
| ATOM | 1652 | O | PHE | A | 219 | 25.390 | 36.490 | 22.416 | 1.00 | 21.88 | O |
| ATOM | 1653 | CB | PHE | A | 219 | 23.005 | 38.484 | 22.820 | 1.00 | 20.94 | C |
| ATOM | 1654 | CG | PHE | A | 219 | 21.541 | 38.617 | 23.106 | 1.00 | 21.13 | C |
| ATOM | 1655 | CD1 | PHE | A | 219 | 20.907 | 37.779 | 23.995 | 1.00 | 21.92 | C |
| ATOM | 1656 | CD2 | PHE | A | 219 | 20.785 | 39.589 | 22.476 | 1.00 | 24.21 | C |
| ATOM | 1657 | CE1 | PHE | A | 219 | 19.563 | 37.915 | 24.250 | 1.00 | 21.95 | C |
| ATOM | 1658 | CE2 | PHE | A | 219 | 19.442 | 39.724 | 22.735 | 1.00 | 22.06 | C |
| ATOM | 1659 | CZ | PHE | A | 219 | 18.840 | 38.904 | 23.621 | 1.00 | 23.11 | C |
| ATOM | 1660 | N | PRO | A | 220 | 25.512 | 37.877 | 20.662 | 1.00 | 22.38 | N |
| ATOM | 1661 | CA | PRO | A | 220 | 26.962 | 37.744 | 20.557 | 1.00 | 22.81 | C |
| ATOM | 1662 | C | PRO | A | 220 | 27.683 | 38.287 | 21.793 | 1.00 | 22.78 | C |
| ATOM | 1663 | O | PRO | A | 220 | 27.173 | 39.123 | 22.564 | 1.00 | 22.88 | O |
| ATOM | 1664 | CB | PRO | A | 220 | 27.335 | 38.561 | 19.317 | 1.00 | 22.81 | C |
| ATOM | 1665 | CG | PRO | A | 220 | 26.005 | 39.005 | 18.685 | 1.00 | 23.68 | C |
| ATOM | 1666 | CD | PRO | A | 220 | 24.940 | 38.792 | 19.663 | 1.00 | 22.86 | C |
| ATOM | 1667 | N | PRO | A | 221 | 28.885 | 37.774 | 21.999 | 1.00 | 22.84 | N |
| ATOM | 1668 | CA | PRO | A | 221 | 29.724 | 38.204 | 23.124 | 1.00 | 22.73 | C |
| ATOM | 1669 | C | PRO | A | 221 | 29.976 | 39.714 | 23.143 | 1.00 | 22.28 | C |
| ATOM | 1670 | O | PRO | A | 221 | 30.192 | 40.279 | 24.212 | 1.00 | 21.03 | O |
| ATOM | 1671 | CB | PRO | A | 221 | 31.030 | 37.455 | 22.892 | 1.00 | 22.78 | C |
| ATOM | 1672 | CG | PRO | A | 221 | 30.644 | 36.296 | 22.026 | 1.00 | 23.22 | C |
| ATOM | 1673 | CD | PRO | A | 221 | 29.521 | 36.733 | 21.174 | 1.00 | 22.58 | C |
| ATOM | 1674 | N | ASP | A | 222 | 29.897 | 40.378 | 21.993 | 1.00 | 22.60 | N |
| ATOM | 1675 | CA | ASP | A | 222 | 30.172 | 41.821 | 21.965 | 1.00 | 22.84 | C |
| ATOM | 1676 | C | ASP | A | 222 | 28.996 | 42.623 | 22.493 | 1.00 | 23.36 | C |
| ATOM | 1677 | O | ASP | A | 222 | 29.031 | 43.847 | 22.500 | 1.00 | 24.43 | O |
| ATOM | 1678 | CB | ASP | A | 222 | 30.638 | 42.308 | 20.579 | 1.00 | 22.47 | C |
| ATOM | 1679 | CG | ASP | A | 222 | 29.502 | 42.389 | 19.537 | 1.00 | 25.07 | C |
| ATOM | 1680 | OD1 | ASP | A | 222 | 28.355 | 41.942 | 19.764 | 1.00 | 25.24 | O |
| ATOM | 1681 | OD2 | ASP | A | 222 | 29.690 | 42.876 | 18.410 | 1.00 | 29.46 | O |
| ATOM | 1682 | N | GLN | A | 223 | 27.940 | 41.940 | 22.926 | 1.00 | 23.79 | N |
| ATOM | 1683 | CA | GLN | A | 223 | 26.826 | 42.624 | 23.565 | 1.00 | 23.85 | C |
| ATOM | 1684 | C | GLN | A | 223 | 26.942 | 42.570 | 25.114 | 1.00 | 23.37 | C |
| ATOM | 1685 | O | GLN | A | 223 | 25.986 | 42.875 | 25.850 | 1.00 | 23.78 | O |
| ATOM | 1686 | CB | GLN | A | 223 | 25.510 | 42.084 | 23.007 | 1.00 | 24.80 | C |
| ATOM | 1687 | CG | GLN | A | 223 | 25.217 | 42.672 | 21.550 | 1.00 | 28.46 | C |
| ATOM | 1688 | CD | GLN | A | 223 | 23.786 | 42.471 | 21.094 | 1.00 | 32.35 | C |
| ATOM | 1689 | OE1 | GLN | A | 223 | 22.861 | 42.619 | 21.893 | 1.00 | 36.73 | O |
| ATOM | 1690 | NE2 | GLN | A | 223 | 23.592 | 42.105 | 19.815 | 1.00 | 33.48 | N |
| ATOM | 1691 | N | PHE | A | 224 | 28.111 | 42.167 | 25.601 | 1.00 | 21.59 | N |
| ATOM | 1692 | CA | PHE | A | 224 | 28.394 | 42.195 | 27.035 | 1.00 | 21.84 | C |
| ATOM | 1693 | C | PHE | A | 224 | 27.888 | 43.509 | 27.706 | 1.00 | 21.56 | C |
| ATOM | 1694 | O | PHE | A | 224 | 27.233 | 43.455 | 28.738 | 1.00 | 20.27 | O |
| ATOM | 1695 | CB | PHE | A | 224 | 29.917 | 42.068 | 27.271 | 1.00 | 21.34 | C |
| ATOM | 1696 | CG | PHE | A | 224 | 30.309 | 41.943 | 28.732 | 1.00 | 22.22 | C |
| ATOM | 1697 | CD1 | PHE | A | 224 | 30.449 | 43.071 | 29.540 | 1.00 | 21.80 | C |
| ATOM | 1698 | CD2 | PHE | A | 224 | 30.583 | 40.723 | 29.279 | 1.00 | 20.92 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1699 | CE1 | PHE | A | 224 | 30.842 | 42.945 | 30.868 | 1.00 | 22.58 | C |
| ATOM | 1700 | CE2 | PHE | A | 224 | 30.979 | 40.593 | 30.587 | 1.00 | 22.14 | C |
| ATOM | 1701 | CZ | PHE | A | 224 | 31.087 | 41.725 | 31.394 | 1.00 | 22.16 | C |
| ATOM | 1702 | N | GLU | A | 225 | 28.190 | 44.665 | 27.106 | 1.00 | 22.03 | N |
| ATOM | 1703 | CA | GLU | A | 225 | 27.813 | 45.963 | 27.677 | 1.00 | 23.55 | C |
| ATOM | 1704 | C | GLU | A | 225 | 26.322 | 46.216 | 27.764 | 1.00 | 23.06 | C |
| ATOM | 1705 | O | GLU | A | 225 | 25.907 | 47.129 | 28.483 | 1.00 | 22.10 | O |
| ATOM | 1706 | CB | GLU | A | 225 | 28.396 | 47.111 | 26.856 | 1.00 | 24.92 | C |
| ATOM | 1707 | CG | GLU | A | 225 | 29.897 | 47.228 | 27.013 | 1.00 | 30.17 | C |
| ATOM | 1708 | CD | GLU | A | 225 | 30.386 | 48.632 | 27.280 | 1.00 | 36.52 | C |
| ATOM | 1709 | OE1 | GLU | A | 225 | 29.901 | 49.319 | 28.242 | 1.00 | 40.52 | O |
| ATOM | 1710 | OE2 | GLU | A | 225 | 31.310 | 49.028 | 26.532 | 1.00 | 41.63 | O |
| ATOM | 1711 | N | CYS | A | 226 | 25.532 | 45.456 | 27.003 | 1.00 | 22.07 | N |
| ATOM | 1712 | CA | CYS | A | 226 | 24.087 | 45.619 | 27.027 | 1.00 | 22.09 | C |
| ATOM | 1713 | C | CYS | A | 226 | 23.372 | 44.631 | 27.935 | 1.00 | 21.89 | C |
| ATOM | 1714 | O | CYS | A | 226 | 22.170 | 44.781 | 28.162 | 1.00 | 20.73 | O |
| ATOM | 1715 | CB | CYS | A | 226 | 23.523 | 45.416 | 25.630 | 1.00 | 22.22 | C |
| ATOM | 1716 | SG | CYS | A | 226 | 24.206 | 46.488 | 24.368 | 1.00 | 22.59 | S |
| ATOM | 1717 | N | LEU | A | 227 | 24.102 | 43.633 | 28.451 | 1.00 | 22.08 | N |
| ATOM | 1718 | CA | LEU | A | 227 | 23.467 | 42.529 | 29.169 | 1.00 | 22.08 | C |
| ATOM | 1719 | C | LEU | A | 227 | 23.771 | 42.393 | 30.657 | 1.00 | 21.99 | C |
| ATOM | 1720 | O | LEU | A | 227 | 23.118 | 41.611 | 31.373 | 1.00 | 22.28 | O |
| ATOM | 1721 | CB | LEU | A | 227 | 23.751 | 41.244 | 28.418 | 1.00 | 22.29 | C |
| ATOM | 1722 | CG | LEU | A | 227 | 22.874 | 41.185 | 27.158 | 1.00 | 23.54 | C |
| ATOM | 1723 | CD1 | LEU | A | 227 | 23.428 | 40.186 | 26.144 | 1.00 | 23.51 | C |
| ATOM | 1724 | CD2 | LEU | A | 227 | 21.423 | 40.819 | 27.544 | 1.00 | 24.49 | C |
| ATOM | 1725 | N | TYR | A | 228 | 24.763 | 43.140 | 31.109 | 1.00 | 20.87 | N |
| ATOM | 1726 | CA | TYR | A | 228 | 24.996 | 43.320 | 32.521 | 1.00 | 21.33 | C |
| ATOM | 1727 | C | TYR | A | 228 | 25.018 | 42.057 | 33.382 | 1.00 | 21.27 | C |
| ATOM | 1728 | O | TYR | A | 228 | 24.205 | 41.920 | 34.301 | 1.00 | 21.72 | O |
| ATOM | 1729 | CB | TYR | A | 228 | 23.957 | 44.311 | 33.077 | 1.00 | 20.92 | C |
| ATOM | 1730 | CG | TYR | A | 228 | 23.949 | 45.649 | 32.339 | 1.00 | 20.91 | C |
| ATOM | 1731 | CD1 | TYR | A | 228 | 24.768 | 46.677 | 32.739 | 1.00 | 18.87 | C |
| ATOM | 1732 | CD2 | TYR | A | 228 | 23.122 | 45.862 | 31.232 | 1.00 | 20.51 | C |
| ATOM | 1733 | CE1 | TYR | A | 228 | 24.780 | 47.912 | 32.076 | 1.00 | 20.36 | C |
| ATOM | 1734 | CE2 | TYR | A | 228 | 23.117 | 47.074 | 30.561 | 1.00 | 21.07 | C |
| ATOM | 1735 | CZ | TYR | A | 228 | 23.931 | 48.113 | 31.000 | 1.00 | 20.84 | C |
| ATOM | 1736 | OH | TYR | A | 228 | 23.947 | 49.325 | 30.336 | 1.00 | 19.16 | O |
| ATOM | 1737 | N | PRO | A | 229 | 25.985 | 41.175 | 33.141 | 1.00 | 20.77 | N |
| ATOM | 1738 | CA | PRO | A | 229 | 26.128 | 39.971 | 33.966 | 1.00 | 21.05 | C |
| ATOM | 1739 | C | PRO | A | 229 | 26.428 | 40.332 | 35.408 | 1.00 | 20.08 | C |
| ATOM | 1740 | O | PRO | A | 229 | 27.021 | 41.379 | 35.675 | 1.00 | 20.20 | O |
| ATOM | 1741 | CB | PRO | A | 229 | 27.360 | 39.271 | 33.363 | 1.00 | 20.51 | C |
| ATOM | 1742 | CG | PRO | A | 229 | 28.084 | 40.340 | 32.651 | 1.00 | 21.64 | C |
| ATOM | 1743 | CD | PRO | A | 229 | 27.025 | 41.241 | 32.105 | 1.00 | 20.97 | C |
| ATOM | 1744 | N | TYR | A | 230 | 25.988 | 39.490 | 36.326 | 1.00 | 19.73 | N |
| ATOM | 1745 | CA | TYR | A | 230 | 26.282 | 39.656 | 37.724 | 1.00 | 18.80 | C |
| ATOM | 1746 | C | TYR | A | 230 | 27.809 | 39.657 | 37.947 | 1.00 | 18.61 | C |
| ATOM | 1747 | O | TYR | A | 230 | 28.575 | 39.250 | 37.094 | 1.00 | 18.26 | O |
| ATOM | 1748 | CB | TYR | A | 230 | 25.669 | 38.507 | 38.520 | 1.00 | 18.86 | C |
| ATOM | 1749 | CG | TYR | A | 230 | 24.172 | 38.597 | 38.725 | 1.00 | 19.28 | C |
| ATOM | 1750 | CD1 | TYR | A | 230 | 23.297 | 38.110 | 37.760 | 1.00 | 18.53 | C |
| ATOM | 1751 | CD2 | TYR | A | 230 | 23.629 | 39.172 | 39.885 | 1.00 | 19.38 | C |
| ATOM | 1752 | CE1 | TYR | A | 230 | 21.932 | 38.161 | 37.935 | 1.00 | 18.86 | C |
| ATOM | 1753 | CE2 | TYR | A | 230 | 22.234 | 39.222 | 40.076 | 1.00 | 19.53 | C |
| ATOM | 1754 | CZ | TYR | A | 230 | 21.404 | 38.719 | 39.073 | 1.00 | 20.93 | C |
| ATOM | 1755 | OH | TYR | A | 230 | 20.034 | 38.771 | 39.176 | 1.00 | 23.69 | O |
| ATOM | 1756 | N | PRO | A | 231 | 28.251 | 40.137 | 39.098 | 1.00 | 18.40 | N |
| ATOM | 1757 | CA | PRO | A | 231 | 29.651 | 39.983 | 39.476 | 1.00 | 18.58 | C |
| ATOM | 1758 | C | PRO | A | 231 | 30.070 | 38.507 | 39.399 | 1.00 | 19.41 | C |
| ATOM | 1759 | O | PRO | A | 231 | 29.240 | 37.624 | 39.654 | 1.00 | 18.89 | O |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1760 | CB | PRO | A | 231 | 29.675 | 40.477 | 40.931 | 1.00 | 18.95 | C |
| ATOM | 1761 | CG | PRO | A | 231 | 28.542 | 41.507 | 41.001 | 1.00 | 19.02 | C |
| ATOM | 1762 | CD | PRO | A | 231 | 27.460 | 40.868 | 40.105 | 1.00 | 18.02 | C |
| ATOM | 1763 | N | VAL | A | 232 | 31.335 | 38.248 | 39.071 | 1.00 | 19.55 | N |
| ATOM | 1764 | CA | VAL | A | 232 | 31.826 | 36.884 | 38.969 | 1.00 | 20.65 | C |
| ATOM | 1765 | C | VAL | A | 232 | 31.640 | 36.034 | 40.236 | 1.00 | 20.79 | C |
| ATOM | 1766 | O | VAL | A | 232 | 31.379 | 34.838 | 40.145 | 1.00 | 21.82 | O |
| ATOM | 1767 | CB | VAL | A | 232 | 33.318 | 36.869 | 38.545 | 1.00 | 20.71 | C |
| ATOM | 1768 | CG1 | VAL | A | 232 | 33.945 | 35.524 | 38.807 | 1.00 | 21.96 | C |
| ATOM | 1769 | CG2 | VAL | A | 232 | 33.452 | 37.225 | 37.075 | 1.00 | 20.83 | C |
| ATOM | 1770 | N | HIS | A | 233 | 31.770 | 36.639 | 41.409 | 1.00 | 20.87 | N |
| ATOM | 1771 | CA | HIS | A | 233 | 31.643 | 35.907 | 42.661 | 1.00 | 20.70 | C |
| ATOM | 1772 | C | HIS | A | 233 | 30.203 | 35.739 | 43.168 | 1.00 | 20.59 | C |
| ATOM | 1773 | O | HIS | A | 233 | 29.940 | 35.010 | 44.119 | 1.00 | 20.49 | O |
| ATOM | 1774 | CB | HIS | A | 233 | 32.482 | 36.593 | 43.706 | 1.00 | 20.63 | C |
| ATOM | 1775 | CG | HIS | A | 233 | 33.948 | 36.529 | 43.426 | 1.00 | 21.92 | C |
| ATOM | 1776 | ND1 | HIS | A | 233 | 34.659 | 37.595 | 42.913 | 1.00 | 22.17 | N |
| ATOM | 1777 | CD2 | HIS | A | 233 | 34.843 | 35.527 | 43.610 | 1.00 | 22.03 | C |
| ATOM | 1778 | CE1 | HIS | A | 233 | 35.929 | 37.249 | 42.793 | 1.00 | 23.69 | C |
| ATOM | 1779 | NE2 | HIS | A | 233 | 36.066 | 35.998 | 43.203 | 1.00 | 23.04 | N |
| ATOM | 1780 | N | HIS | A | 234 | 29.273 | 36.433 | 42.543 | 1.00 | 20.53 | N |
| ATOM | 1781 | CA | HIS | A | 234 | 27.869 | 36.251 | 42.857 | 1.00 | 20.60 | C |
| ATOM | 1782 | C | HIS | A | 234 | 27.388 | 34.895 | 42.306 | 1.00 | 20.45 | C |
| ATOM | 1783 | O | HIS | A | 234 | 27.873 | 34.428 | 41.291 | 1.00 | 19.86 | O |
| ATOM | 1784 | CB | HIS | A | 234 | 27.088 | 37.359 | 42.206 | 1.00 | 20.65 | C |
| ATOM | 1785 | CG | HIS | A | 234 | 25.661 | 37.441 | 42.625 | 1.00 | 20.68 | C |
| ATOM | 1786 | ND1 | HIS | A | 234 | 24.667 | 36.700 | 42.021 | 1.00 | 21.46 | N |
| ATOM | 1787 | CD2 | HIS | A | 234 | 25.044 | 38.249 | 43.518 | 1.00 | 20.20 | C |
| ATOM | 1788 | CE1 | HIS | A | 234 | 23.504 | 37.013 | 42.563 | 1.00 | 21.99 | C |
| ATOM | 1789 | NE2 | HIS | A | 234 | 23.707 | 37.951 | 43.473 | 1.00 | 21.29 | N |
| ATOM | 1790 | N | PRO | A | 235 | 26.463 | 34.261 | 43.007 | 1.00 | 20.40 | N |
| ATOM | 1791 | CA | PRO | A | 235 | 25.888 | 32.993 | 42.572 | 1.00 | 20.85 | C |
| ATOM | 1792 | C | PRO | A | 235 | 25.360 | 33.021 | 41.152 | 1.00 | 21.20 | C |
| ATOM | 1793 | O | PRO | A | 235 | 25.437 | 31.984 | 40.502 | 1.00 | 20.43 | O |
| ATOM | 1794 | CB | PRO | A | 235 | 24.756 | 32.771 | 43.575 | 1.00 | 21.58 | C |
| ATOM | 1795 | CG | PRO | A | 235 | 25.273 | 33.452 | 44.826 | 1.00 | 20.78 | C |
| ATOM | 1796 | CD | PRO | A | 235 | 25.941 | 34.685 | 44.317 | 1.00 | 20.56 | C |
| ATOM | 1797 | N | CYS | A | 236 | 24.905 | 34.173 | 40.663 | 1.00 | 20.46 | N |
| ATOM | 1798 | CA | CYS | A | 236 | 24.379 | 34.235 | 39.308 | 1.00 | 20.63 | C |
| ATOM | 1799 | C | CYS | A | 236 | 25.430 | 34.707 | 38.301 | 1.00 | 20.58 | C |
| ATOM | 1800 | O | CYS | A | 236 | 25.110 | 35.283 | 37.258 | 1.00 | 21.60 | O |
| ATOM | 1801 | CB | CYS | A | 236 | 23.114 | 35.084 | 39.268 | 1.00 | 20.06 | C |
| ATOM | 1802 | SG | CYS | A | 236 | 21.824 | 34.377 | 40.326 | 1.00 | 21.70 | S |
| ATOM | 1803 | N | ASP | A | 237 | 26.693 | 34.474 | 38.629 | 1.00 | 20.17 | N |
| ATOM | 1804 | CA | ASP | A | 237 | 27.785 | 34.632 | 37.679 | 1.00 | 19.98 | C |
| ATOM | 1805 | C | ASP | A | 237 | 27.381 | 34.050 | 36.313 | 1.00 | 19.79 | C |
| ATOM | 1806 | O | ASP | A | 237 | 26.830 | 32.950 | 36.234 | 1.00 | 19.19 | O |
| ATOM | 1807 | CB | ASP | A | 237 | 28.997 | 33.872 | 38.200 | 1.00 | 19.91 | C |
| ATOM | 1808 | CG | ASP | A | 237 | 30.209 | 33.968 | 37.290 | 1.00 | 21.43 | C |
| ATOM | 1809 | OD1 | ASP | A | 237 | 30.407 | 35.010 | 36.546 | 1.00 | 18.96 | O |
| ATOM | 1810 | OD2 | ASP | A | 237 | 31.039 | 33.017 | 37.288 | 1.00 | 18.57 | O |
| ATOM | 1811 | N | ARG | A | 238 | 27.664 | 34.812 | 35.263 | 1.00 | 20.18 | N |
| ATOM | 1812 | CA | ARG | A | 238 | 27.365 | 34.473 | 33.865 | 1.00 | 21.48 | C |
| ATOM | 1813 | C | ARG | A | 238 | 25.905 | 34.713 | 33.444 | 1.00 | 20.90 | C |
| ATOM | 1814 | O | ARG | A | 238 | 25.600 | 34.619 | 32.269 | 1.00 | 21.92 | O |
| ATOM | 1815 | CB | ARG | A | 238 | 27.765 | 33.024 | 33.531 | 1.00 | 21.70 | C |
| ATOM | 1816 | CG | ARG | A | 238 | 29.245 | 32.739 | 33.699 | 1.00 | 22.10 | C |
| ATOM | 1817 | CD | ARG | A | 238 | 29.612 | 31.313 | 33.329 | 1.00 | 23.08 | C |
| ATOM | 1818 | NE | ARG | A | 238 | 28.988 | 30.409 | 34.278 | 1.00 | 25.97 | N |
| ATOM | 1819 | CZ | ARG | A | 238 | 27.863 | 29.725 | 34.066 | 1.00 | 27.01 | C |
| ATOM | 1820 | NH1 | ARG | A | 238 | 27.208 | 29.799 | 32.904 | 1.00 | 24.08 | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1821 | NH2 | ARG | A | 238 | 27.399 | 28.949 | 35.036 | 1.00 | 27.47 | N |
| ATOM | 1822 | N | GLN | A | 239 | 25.021 | 35.028 | 34.375 | 1.00 | 20.56 | N |
| ATOM | 1823 | CA | GLN | A | 239 | 23.641 | 35.334 | 34.014 | 1.00 | 21.11 | C |
| ATOM | 1824 | C | GLN | A | 239 | 23.459 | 36.865 | 33.920 | 1.00 | 20.84 | C |
| ATOM | 1825 | O | GLN | A | 239 | 24.145 | 37.624 | 34.610 | 1.00 | 21.25 | O |
| ATOM | 1826 | CB | GLN | A | 239 | 22.646 | 34.776 | 35.027 | 1.00 | 20.14 | C |
| ATOM | 1827 | CG | GLN | A | 239 | 23.052 | 33.505 | 35.726 | 1.00 | 22.87 | C |
| ATOM | 1828 | CD | GLN | A | 239 | 23.281 | 32.320 | 34.807 | 1.00 | 23.97 | C |
| ATOM | 1829 | OE1 | GLN | A | 239 | 22.367 | 31.842 | 34.132 | 1.00 | 23.63 | O |
| ATOM | 1830 | NE2 | GLN | A | 239 | 24.502 | 31.834 | 34.796 | 1.00 | 24.34 | N |
| ATOM | 1831 | N | SER | A | 240 | 22.541 | 37.307 | 33.071 | 1.00 | 20.31 | N |
| ATOM | 1832 | CA | SER | A | 240 | 22.246 | 38.725 | 32.926 | 1.00 | 19.92 | C |
| ATOM | 1833 | C | SER | A | 240 | 21.448 | 39.218 | 34.119 | 1.00 | 20.07 | C |
| ATOM | 1834 | O | SER | A | 240 | 20.538 | 38.533 | 34.564 | 1.00 | 19.79 | O |
| ATOM | 1835 | CB | SER | A | 240 | 21.384 | 38.953 | 31.700 | 1.00 | 19.45 | C |
| ATOM | 1836 | OG | SER | A | 240 | 21.018 | 40.312 | 31.564 | 1.00 | 20.53 | O |
| ATOM | 1837 | N | GLN | A | 241 | 21.763 | 40.408 | 34.623 | 1.00 | 19.46 | N |
| ATOM | 1838 | CA | GLN | A | 241 | 20.962 | 40.988 | 35.701 | 1.00 | 20.32 | C |
| ATOM | 1839 | C | GLN | A | 241 | 19.657 | 41.569 | 35.175 | 1.00 | 20.51 | C |
| ATOM | 1840 | O | GLN | A | 241 | 18.808 | 41.956 | 35.959 | 1.00 | 21.06 | O |
| ATOM | 1841 | CB | GLN | A | 241 | 21.697 | 42.141 | 36.417 | 1.00 | 20.15 | C |
| ATOM | 1842 | CG | GLN | A | 241 | 22.910 | 41.749 | 37.230 | 1.00 | 21.41 | C |
| ATOM | 1843 | CD | GLN | A | 241 | 23.690 | 42.980 | 37.695 | 1.00 | 22.76 | C |
| ATOM | 1844 | OE1 | GLN | A | 241 | 23.455 | 43.481 | 38.775 | 1.00 | 24.42 | O |
| ATOM | 1845 | NE2 | GLN | A | 241 | 24.585 | 43.465 | 36.871 | 1.00 | 21.93 | N |
| ATOM | 1846 | N | VAL | A | 242 | 19.489 | 41.678 | 33.862 | 1.00 | 20.66 | N |
| ATOM | 1847 | CA | VAL | A | 242 | 18.309 | 42.355 | 33.372 | 1.00 | 20.76 | C |
| ATOM | 1848 | C | VAL | A | 242 | 17.089 | 41.465 | 33.391 | 1.00 | 21.26 | C |
| ATOM | 1849 | O | VAL | A | 242 | 17.119 | 40.352 | 32.871 | 1.00 | 21.01 | O |
| ATOM | 1850 | CB | VAL | A | 242 | 18.476 | 42.813 | 31.909 | 1.00 | 20.97 | C |
| ATOM | 1851 | CG1 | VAL | A | 242 | 17.194 | 43.502 | 31.431 | 1.00 | 21.21 | C |
| ATOM | 1852 | CG2 | VAL | A | 242 | 19.687 | 43.704 | 31.716 | 1.00 | 18.95 | C |
| ATOM | 1853 | N | ASP | A | 243 | 16.001 | 41.960 | 33.958 | 1.00 | 21.16 | N |
| ATOM | 1854 | CA | ASP | A | 243 | 14.730 | 41.223 | 33.907 | 1.00 | 21.36 | C |
| ATOM | 1855 | C | ASP | A | 243 | 14.091 | 41.523 | 32.552 | 1.00 | 21.20 | C |
| ATOM | 1856 | O | ASP | A | 243 | 13.566 | 42.631 | 32.310 | 1.00 | 19.97 | O |
| ATOM | 1857 | CB | ASP | A | 243 | 13.840 | 41.682 | 35.054 | 1.00 | 21.65 | C |
| ATOM | 1858 | CG | ASP | A | 243 | 12.474 | 41.051 | 35.037 | 1.00 | 22.45 | C |
| ATOM | 1859 | OD1 | ASP | A | 243 | 12.122 | 40.338 | 34.070 | 1.00 | 25.16 | O |
| ATOM | 1860 | OD2 | ASP | A | 243 | 11.671 | 41.232 | 35.978 | 1.00 | 25.29 | O |
| ATOM | 1861 | N | PHE | A | 244 | 14.182 | 40.554 | 31.650 | 1.00 | 21.28 | N |
| ATOM | 1862 | CA | PHE | A | 244 | 13.687 | 40.733 | 30.291 | 1.00 | 21.65 | C |
| ATOM | 1863 | C | PHE | A | 244 | 12.202 | 41.074 | 30.274 | 1.00 | 22.36 | C |
| ATOM | 1864 | O | PHE | A | 244 | 11.733 | 41.653 | 29.304 | 1.00 | 22.09 | O |
| ATOM | 1865 | CB | PHE | A | 244 | 13.915 | 39.478 | 29.442 | 1.00 | 22.22 | C |
| ATOM | 1866 | CG | PHE | A | 244 | 15.284 | 39.370 | 28.815 | 1.00 | 21.43 | C |
| ATOM | 1867 | CD1 | PHE | A | 244 | 16.414 | 39.800 | 29.465 | 1.00 | 20.12 | C |
| ATOM | 1868 | CD2 | PHE | A | 244 | 15.422 | 38.778 | 27.575 | 1.00 | 21.05 | C |
| ATOM | 1869 | CE1 | PHE | A | 244 | 17.655 | 39.671 | 28.873 | 1.00 | 20.83 | C |
| ATOM | 1870 | CE2 | PHE | A | 244 | 16.645 | 38.643 | 26.993 | 1.00 | 21.47 | C |
| ATOM | 1871 | CZ | PHE | A | 244 | 17.767 | 39.104 | 27.633 | 1.00 | 20.74 | C |
| ATOM | 1872 | N | ASP | A | 245 | 11.464 | 40.696 | 31.322 | 1.00 | 23.26 | N |
| ATOM | 1873 | CA | ASP | A | 245 | 10.035 | 40.973 | 31.393 | 1.00 | 24.31 | C |
| ATOM | 1874 | C | ASP | A | 245 | 9.756 | 42.401 | 31.877 | 1.00 | 25.05 | C |
| ATOM | 1875 | O | ASP | A | 245 | 8.679 | 42.916 | 31.646 | 1.00 | 24.27 | O |
| ATOM | 1876 | CB | ASP | A | 245 | 9.333 | 40.004 | 32.348 | 1.00 | 24.79 | C |
| ATOM | 1877 | CG | ASP | A | 245 | 9.397 | 38.571 | 31.887 | 1.00 | 25.46 | C |
| ATOM | 1878 | OD1 | ASP | A | 245 | 9.409 | 38.342 | 30.663 | 1.00 | 27.47 | O |
| ATOM | 1879 | OD2 | ASP | A | 245 | 9.445 | 37.610 | 32.678 | 1.00 | 25.22 | O |
| ATOM | 1880 | N | ASN | A | 246 | 10.702 | 43.006 | 32.589 | 1.00 | 25.30 | N |
| ATOM | 1881 | CA | ASN | A | 246 | 10.531 | 44.365 | 33.099 | 1.00 | 26.37 | C |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1882 | C | ASN A 246 | 11.876 | 45.054 | 33.204 | 1.00 | 25.61 | C |
| ATOM | 1883 | O | ASN A 246 | 12.436 | 45.192 | 34.282 | 1.00 | 26.05 | O |
| ATOM | 1884 | CB | ASN A 246 | 9.871 | 44.360 | 34.472 | 1.00 | 26.89 | C |
| ATOM | 1885 | CG | ASN A 246 | 9.545 | 45.770 | 34.958 | 1.00 | 30.93 | C |
| ATOM | 1886 | OD1 | ASN A 246 | 9.353 | 46.701 | 34.150 | 1.00 | 35.10 | O |
| ATOM | 1887 | ND2 | ASN A 246 | 9.493 | 45.943 | 36.281 | 1.00 | 35.04 | N |
| ATOM | 1888 | N | PRO A 247 | 12.415 | 45.450 | 32.068 | 1.00 | 24.71 | N |
| ATOM | 1889 | CA | PRO A 247 | 13.775 | 45.979 | 32.026 | 1.00 | 24.24 | C |
| ATOM | 1890 | C | PRO A 247 | 13.909 | 47.352 | 32.684 | 1.00 | 24.48 | C |
| ATOM | 1891 | O | PRO A 247 | 13.189 | 48.296 | 32.374 | 1.00 | 23.54 | O |
| ATOM | 1892 | CB | PRO A 247 | 14.109 | 46.036 | 30.538 | 1.00 | 24.23 | C |
| ATOM | 1893 | CG | PRO A 247 | 12.900 | 45.524 | 29.803 | 1.00 | 25.13 | C |
| ATOM | 1894 | CD | PRO A 247 | 11.769 | 45.385 | 30.752 | 1.00 | 24.61 | C |
| ATOM | 1895 | N | ASP A 248 | 14.867 | 47.437 | 33.593 | 1.00 | 24.04 | N |
| ATOM | 1896 | CA | ASP A 248 | 15.140 | 48.656 | 34.285 | 1.00 | 24.53 | C |
| ATOM | 1897 | C | ASP A 248 | 16.206 | 49.440 | 33.496 | 1.00 | 24.15 | C |
| ATOM | 1898 | O | ASP A 248 | 17.410 | 49.221 | 33.629 | 1.00 | 23.11 | O |
| ATOM | 1899 | CB | ASP A 248 | 15.609 | 48.312 | 35.689 | 1.00 | 24.75 | C |
| ATOM | 1900 | CG | ASP A 248 | 15.731 | 49.512 | 36.554 | 1.00 | 26.08 | C |
| ATOM | 1901 | OD1 | ASP A 248 | 15.956 | 50.616 | 36.009 | 1.00 | 27.08 | O |
| ATOM | 1902 | OD2 | ASP A 248 | 15.623 | 49.439 | 37.797 | 1.00 | 30.33 | O |
| ATOM | 1903 | N | TYR A 249 | 15.735 | 50.329 | 32.642 | 1.00 | 24.42 | N |
| ATOM | 1904 | CA | TYR A 249 | 16.612 | 51.129 | 31.807 | 1.00 | 25.30 | C |
| ATOM | 1905 | C | TYR A 249 | 17.462 | 52.136 | 32.589 | 1.00 | 26.13 | C |
| ATOM | 1906 | O | TYR A 249 | 18.495 | 52.584 | 32.083 | 1.00 | 26.46 | O |
| ATOM | 1907 | CB | TYR A 249 | 15.796 | 51.826 | 30.713 | 1.00 | 25.41 | C |
| ATOM | 1908 | CG | TYR A 249 | 15.119 | 50.853 | 29.768 | 1.00 | 22.90 | C |
| ATOM | 1909 | CD1 | TYR A 249 | 15.844 | 49.873 | 29.130 | 1.00 | 22.91 | C |
| ATOM | 1910 | CD2 | TYR A 249 | 13.760 | 50.923 | 29.519 | 1.00 | 22.21 | C |
| ATOM | 1911 | CE1 | TYR A 249 | 15.238 | 48.964 | 28.271 | 1.00 | 22.19 | C |
| ATOM | 1912 | CE2 | TYR A 249 | 13.144 | 50.023 | 28.660 | 1.00 | 21.56 | C |
| ATOM | 1913 | CZ | TYR A 249 | 13.895 | 49.044 | 28.046 | 1.00 | 21.23 | C |
| ATOM | 1914 | OH | TYR A 249 | 13.304 | 48.163 | 27.173 | 1.00 | 23.38 | O |
| ATOM | 1915 | N | GLU A 250 | 17.071 | 52.465 | 33.822 | 1.00 | 26.65 | N |
| ATOM | 1916 | CA | GLU A 250 | 17.894 | 53.365 | 34.640 | 1.00 | 27.47 | C |
| ATOM | 1917 | C | GLU A 250 | 19.161 | 52.651 | 35.086 | 1.00 | 26.52 | C |
| ATOM | 1918 | O | GLU A 250 | 20.238 | 53.224 | 35.086 | 1.00 | 27.17 | O |
| ATOM | 1919 | CB | GLU A 250 | 17.133 | 53.908 | 35.866 | 1.00 | 27.89 | C |
| ATOM | 1920 | CG | GLU A 250 | 15.880 | 54.684 | 35.485 | 1.00 | 32.57 | C |
| ATOM | 1921 | CD | GLU A 250 | 15.258 | 55.459 | 36.631 | 1.00 | 37.09 | C |
| ATOM | 1922 | OE1 | GLU A 250 | 15.809 | 55.491 | 37.753 | 1.00 | 42.28 | O |
| ATOM | 1923 | OE2 | GLU A 250 | 14.198 | 56.055 | 36.399 | 1.00 | 42.29 | O |
| ATOM | 1924 | N | ARG A 251 | 19.042 | 51.399 | 35.490 | 1.00 | 25.57 | N |
| ATOM | 1925 | CA | ARG A 251 | 20.224 | 50.657 | 35.900 | 1.00 | 24.72 | C |
| ATOM | 1926 | C | ARG A 251 | 20.955 | 50.069 | 34.718 | 1.00 | 23.56 | C |
| ATOM | 1927 | O | ARG A 251 | 22.150 | 49.919 | 34.769 | 1.00 | 22.92 | O |
| ATOM | 1928 | CB | ARG A 251 | 19.845 | 49.520 | 36.845 | 1.00 | 25.64 | C |
| ATOM | 1929 | CG | ARG A 251 | 19.435 | 49.957 | 38.255 | 1.00 | 26.79 | C |
| ATOM | 1930 | CD | ARG A 251 | 18.858 | 48.815 | 39.123 | 1.00 | 30.01 | C |
| ATOM | 1931 | NE | ARG A 251 | 19.900 | 47.875 | 39.540 | 1.00 | 31.06 | N |
| ATOM | 1932 | CZ | ARG A 251 | 19.709 | 46.579 | 39.766 | 1.00 | 32.72 | C |
| ATOM | 1933 | NH1 | ARG A 251 | 18.508 | 46.029 | 39.628 | 1.00 | 33.10 | N |
| ATOM | 1934 | NH2 | ARG A 251 | 20.734 | 45.828 | 40.135 | 1.00 | 33.44 | N |
| ATOM | 1935 | N | PHE A 252 | 20.234 | 49.725 | 33.652 | 1.00 | 22.66 | N |
| ATOM | 1936 | CA | PHE A 252 | 20.826 | 49.019 | 32.532 | 1.00 | 21.99 | C |
| ATOM | 1937 | C | PHE A 252 | 20.521 | 49.719 | 31.198 | 1.00 | 21.71 | C |
| ATOM | 1938 | O | PHE A 252 | 19.900 | 49.160 | 30.289 | 1.00 | 21.32 | O |
| ATOM | 1939 | CB | PHE A 252 | 20.261 | 47.610 | 32.519 | 1.00 | 22.03 | C |
| ATOM | 1940 | CG | PHE A 252 | 20.292 | 46.915 | 33.868 | 1.00 | 21.75 | C |
| ATOM | 1941 | CD1 | PHE A 252 | 21.484 | 46.729 | 34.556 | 1.00 | 20.90 | C |
| ATOM | 1942 | CD2 | PHE A 252 | 19.124 | 46.402 | 34.423 | 1.00 | 21.94 | C |

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ATOM   1943  CE1 PHE A 252      21.506  46.040  35.785  1.00 20.51           C
ATOM   1944  CE2 PHE A 252      19.136  45.730  35.662  1.00 21.77           C
ATOM   1945  CZ  PHE A 252      20.320  45.553  36.333  1.00 21.41           C
ATOM   1946  N   PRO A 253      20.989  50.944  31.071  1.00 20.88           N
ATOM   1947  CA  PRO A 253      20.615  51.754  29.909  1.00 20.51           C
ATOM   1948  C   PRO A 253      20.956  51.077  28.578  1.00 20.47           C
ATOM   1949  O   PRO A 253      20.153  51.159  27.656  1.00 20.01           O
ATOM   1950  CB  PRO A 253      21.371  53.077  30.130  1.00 20.00           C
ATOM   1951  CG  PRO A 253      22.538  52.697  31.136  1.00 20.46           C
ATOM   1952  CD  PRO A 253      21.921  51.641  31.994  1.00 20.89           C
ATOM   1953  N   ASN A 254      22.088  50.393  28.455  1.00 20.68           N
ATOM   1954  CA  ASN A 254      22.401  49.805  27.160  1.00 20.72           C
ATOM   1955  C   ASN A 254      21.537  48.601  26.790  1.00 20.29           C
ATOM   1956  O   ASN A 254      21.644  48.068  25.688  1.00 20.03           O
ATOM   1957  CB  ASN A 254      23.882  49.463  27.033  1.00 20.89           C
ATOM   1958  CG  ASN A 254      24.736  50.698  26.899  1.00 22.24           C
ATOM   1959  OD1 ASN A 254      25.532  50.999  27.785  1.00 24.48           O
ATOM   1960  ND2 ASN A 254      24.557  51.446  25.791  1.00 22.23           N
ATOM   1961  N   PHE A 255      20.678  48.160  27.690  1.00 20.01           N
ATOM   1962  CA  PHE A 255      19.781  47.086  27.305  1.00 20.02           C
ATOM   1963  C   PHE A 255      18.855  47.599  26.185  1.00 20.33           C
ATOM   1964  O   PHE A 255      18.224  46.818  25.472  1.00 19.82           O
ATOM   1965  CB  PHE A 255      18.970  46.552  28.484  1.00 19.63           C
ATOM   1966  CG  PHE A 255      18.239  45.318  28.145  1.00 18.96           C
ATOM   1967  CD1 PHE A 255      18.928  44.149  27.930  1.00 19.50           C
ATOM   1968  CD2 PHE A 255      16.889  45.335  27.942  1.00 17.83           C
ATOM   1969  CE1 PHE A 255      18.267  42.997  27.575  1.00 20.08           C
ATOM   1970  CE2 PHE A 255      16.230  44.206  27.561  1.00 17.77           C
ATOM   1971  CZ  PHE A 255      16.912  43.036  27.381  1.00 21.57           C
ATOM   1972  N   GLN A 256      18.788  48.919  26.035  1.00 20.15           N
ATOM   1973  CA  GLN A 256      17.973  49.533  24.986  1.00 20.63           C
ATOM   1974  C   GLN A 256      18.594  49.343  23.591  1.00 20.12           C
ATOM   1975  O   GLN A 256      17.955  49.612  22.592  1.00 19.87           O
ATOM   1976  CB  GLN A 256      17.787  51.036  25.272  1.00 20.67           C
ATOM   1977  CG  GLN A 256      16.744  51.306  26.362  1.00 22.56           C
ATOM   1978  CD  GLN A 256      16.747  52.732  26.888  1.00 22.75           C
ATOM   1979  OE1 GLN A 256      15.727  53.420  26.816  1.00 24.69           O
ATOM   1980  NE2 GLN A 256      17.873  53.172  27.419  1.00 23.90           N
ATOM   1981  N   ASN A 257      19.850  48.915  23.553  1.00 20.07           N
ATOM   1982  CA  ASN A 257      20.583  48.700  22.310  1.00 20.66           C
ATOM   1983  C   ASN A 257      20.778  47.233  21.963  1.00 21.21           C
ATOM   1984  O   ASN A 257      21.446  46.921  20.979  1.00 21.28           O
ATOM   1985  CB  ASN A 257      21.975  49.300  22.420  1.00 20.31           C
ATOM   1986  CG  ASN A 257      21.937  50.757  22.776  1.00 20.83           C
ATOM   1987  OD1 ASN A 257      22.395  51.141  23.850  1.00 20.15           O
ATOM   1988  ND2 ASN A 257      21.366  51.577  21.889  1.00 16.99           N
ATOM   1989  N   VAL A 258      20.218  46.333  22.758  1.00 21.91           N
ATOM   1990  CA  VAL A 258      20.440  44.908  22.532  1.00 23.55           C
ATOM   1991  C   VAL A 258      19.720  44.400  21.284  1.00 24.29           C
ATOM   1992  O   VAL A 258      18.600  44.845  20.947  1.00 24.28           O
ATOM   1993  CB  VAL A 258      20.026  44.110  23.772  1.00 24.18           C
ATOM   1994  CG1 VAL A 258      18.529  43.868  23.785  1.00 23.69           C
ATOM   1995  CG2 VAL A 258      20.761  42.851  23.826  1.00 28.07           C
ATOM   1996  N   VAL A 259      20.381  43.506  20.562  1.00 24.48           N
ATOM   1997  CA  VAL A 259      19.787  42.922  19.364  1.00 25.21           C
ATOM   1998  C   VAL A 259      20.104  41.427  19.331  1.00 25.19           C
ATOM   1999  O   VAL A 259      21.260  41.046  19.333  1.00 25.58           O
ATOM   2000  CB  VAL A 259      20.345  43.551  18.094  1.00 25.37           C
ATOM   2001  CG1 VAL A 259      19.726  42.893  16.882  1.00 27.15           C
ATOM   2002  CG2 VAL A 259      20.074  45.059  18.066  1.00 25.97           C
ATOM   2003  N   GLY A 260      19.068  40.603  19.308  1.00 25.20           N
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2004 | CA | GLY | A | 260 | 19.214 | 39.161 | 19.312 | 1.00 | 25.52 | C |
| ATOM | 2005 | C | GLY | A | 260 | 19.108 | 38.433 | 17.961 | 1.00 | 25.26 | C |
| ATOM | 2006 | O | GLY | A | 260 | 18.762 | 39.016 | 16.914 | 1.00 | 24.66 | O |
| ATOM | 2007 | N | TYR | A | 261 | 19.484 | 37.160 | 18.015 | 1.00 | 24.49 | N |
| ATOM | 2008 | CA | TYR | A | 261 | 19.379 | 36.217 | 16.925 | 1.00 | 25.05 | C |
| ATOM | 2009 | C | TYR | A | 261 | 18.435 | 35.145 | 17.475 | 1.00 | 24.39 | C |
| ATOM | 2010 | O | TYR | A | 261 | 18.671 | 34.620 | 18.552 | 1.00 | 23.82 | O |
| ATOM | 2011 | CB | TYR | A | 261 | 20.730 | 35.574 | 16.627 | 1.00 | 25.82 | C |
| ATOM | 2012 | CG | TYR | A | 261 | 21.748 | 36.476 | 15.965 | 1.00 | 28.98 | C |
| ATOM | 2013 | CD1 | TYR | A | 261 | 21.804 | 36.598 | 14.585 | 1.00 | 35.41 | C |
| ATOM | 2014 | CD2 | TYR | A | 261 | 22.649 | 37.194 | 16.712 | 1.00 | 29.78 | C |
| ATOM | 2015 | CE1 | TYR | A | 261 | 22.737 | 37.429 | 13.976 | 1.00 | 35.73 | C |
| ATOM | 2016 | CE2 | TYR | A | 261 | 23.592 | 37.994 | 16.126 | 1.00 | 32.54 | C |
| ATOM | 2017 | CZ | TYR | A | 261 | 23.643 | 38.116 | 14.768 | 1.00 | 35.98 | C |
| ATOM | 2018 | OH | TYR | A | 261 | 24.580 | 38.959 | 14.202 | 1.00 | 38.02 | O |
| ATOM | 2019 | N | GLU | A | 262 | 17.353 | 34.823 | 16.790 | 1.00 | 24.04 | N |
| ATOM | 2020 | CA | GLU | A | 262 | 16.432 | 33.860 | 17.387 | 1.00 | 23.96 | C |
| ATOM | 2021 | C | GLU | A | 262 | 15.992 | 32.773 | 16.435 | 1.00 | 23.90 | C |
| ATOM | 2022 | O | GLU | A | 262 | 16.116 | 32.890 | 15.213 | 1.00 | 23.56 | O |
| ATOM | 2023 | CB | GLU | A | 262 | 15.224 | 34.553 | 18.020 | 1.00 | 23.70 | C |
| ATOM | 2024 | CG | GLU | A | 262 | 14.029 | 34.782 | 17.127 | 1.00 | 24.33 | C |
| ATOM | 2025 | CD | GLU | A | 262 | 12.829 | 35.382 | 17.870 | 1.00 | 26.49 | C |
| ATOM | 2026 | OE1 | GLU | A | 262 | 12.753 | 36.611 | 18.029 | 1.00 | 27.38 | O |
| ATOM | 2027 | OE2 | GLU | A | 262 | 11.946 | 34.631 | 18.306 | 1.00 | 28.26 | O |
| ATOM | 2028 | N | THR | A | 263 | 15.485 | 31.713 | 17.034 | 1.00 | 23.68 | N |
| ATOM | 2029 | CA | THR | A | 263 | 14.974 | 30.605 | 16.279 | 1.00 | 24.40 | C |
| ATOM | 2030 | C | THR | A | 263 | 14.091 | 29.786 | 17.193 | 1.00 | 24.29 | C |
| ATOM | 2031 | O | THR | A | 263 | 14.131 | 29.936 | 18.423 | 1.00 | 24.53 | O |
| ATOM | 2032 | CB | THR | A | 263 | 16.148 | 29.762 | 15.751 | 1.00 | 24.52 | C |
| ATOM | 2033 | OG1 | THR | A | 263 | 15.684 | 28.839 | 14.762 | 1.00 | 24.43 | O |
| ATOM | 2034 | CG2 | THR | A | 263 | 16.737 | 28.876 | 16.854 | 1.00 | 24.33 | C |
| ATOM | 2035 | N | VAL | A | 264 | 13.263 | 28.954 | 16.593 | 1.00 | 23.62 | N |
| ATOM | 2036 | CA | VAL | A | 264 | 12.500 | 28.019 | 17.370 | 1.00 | 24.01 | C |
| ATOM | 2037 | C | VAL | A | 264 | 12.936 | 26.627 | 16.935 | 1.00 | 24.53 | C |
| ATOM | 2038 | O | VAL | A | 264 | 12.879 | 26.291 | 15.768 | 1.00 | 24.27 | O |
| ATOM | 2039 | CB | VAL | A | 264 | 11.008 | 28.194 | 17.177 | 1.00 | 24.69 | C |
| ATOM | 2040 | CG1 | VAL | A | 264 | 10.256 | 26.958 | 17.712 | 1.00 | 23.69 | C |
| ATOM | 2041 | CG2 | VAL | A | 264 | 10.520 | 29.526 | 17.857 | 1.00 | 23.81 | C |
| ATOM | 2042 | N | VAL | A | 265 | 13.450 | 25.844 | 17.872 | 1.00 | 24.91 | N |
| ATOM | 2043 | CA | VAL | A | 265 | 13.833 | 24.484 | 17.540 | 1.00 | 24.93 | C |
| ATOM | 2044 | C | VAL | A | 265 | 12.792 | 23.470 | 17.967 | 1.00 | 24.20 | C |
| ATOM | 2045 | O | VAL | A | 265 | 12.167 | 23.617 | 19.018 | 1.00 | 24.01 | O |
| ATOM | 2046 | CB | VAL | A | 265 | 15.196 | 24.072 | 18.173 | 1.00 | 25.05 | C |
| ATOM | 2047 | CG1 | VAL | A | 265 | 16.291 | 24.884 | 17.557 | 1.00 | 26.38 | C |
| ATOM | 2048 | CG2 | VAL | A | 265 | 15.190 | 24.164 | 19.702 | 1.00 | 23.59 | C |
| ATOM | 2049 | N | GLY | A | 266 | 12.641 | 22.439 | 17.144 | 1.00 | 23.26 | N |
| ATOM | 2050 | CA | GLY | A | 266 | 11.776 | 21.316 | 17.451 | 1.00 | 23.22 | C |
| ATOM | 2051 | C | GLY | A | 266 | 12.467 | 19.961 | 17.359 | 1.00 | 22.26 | C |
| ATOM | 2052 | O | GLY | A | 266 | 13.661 | 19.872 | 17.131 | 1.00 | 22.37 | O |
| ATOM | 2053 | N | PRO | A | 267 | 11.712 | 18.884 | 17.524 | 1.00 | 21.90 | N |
| ATOM | 2054 | CA | PRO | A | 267 | 12.305 | 17.544 | 17.479 | 1.00 | 21.60 | C |
| ATOM | 2055 | C | PRO | A | 267 | 13.206 | 17.355 | 16.280 | 1.00 | 20.82 | C |
| ATOM | 2056 | O | PRO | A | 267 | 12.768 | 17.588 | 15.169 | 1.00 | 20.29 | O |
| ATOM | 2057 | CB | PRO | A | 267 | 11.086 | 16.622 | 17.364 | 1.00 | 21.36 | C |
| ATOM | 2058 | CG | PRO | A | 267 | 10.023 | 17.330 | 18.028 | 1.00 | 23.23 | C |
| ATOM | 2059 | CD | PRO | A | 267 | 10.254 | 18.831 | 17.753 | 1.00 | 21.99 | C |
| ATOM | 2060 | N | GLY | A | 268 | 14.445 | 16.938 | 16.496 | 1.00 | 20.81 | N |
| ATOM | 2061 | CA | GLY | A | 268 | 15.340 | 16.674 | 15.383 | 1.00 | 20.31 | C |
| ATOM | 2062 | C | GLY | A | 268 | 16.296 | 17.806 | 15.111 | 1.00 | 20.37 | C |
| ATOM | 2063 | O | GLY | A | 268 | 17.333 | 17.605 | 14.476 | 1.00 | 21.79 | O |
| ATOM | 2064 | N | ASP | A | 269 | 15.975 | 19.002 | 15.582 | 1.00 | 19.89 | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2065 | CA | ASP | A | 269 | 16.849 | 20.141 | 15.364 | 1.00 | 19.78 | C |
| ATOM | 2066 | C | ASP | A | 269 | 17.991 | 20.162 | 16.395 | 1.00 | 19.63 | C |
| ATOM | 2067 | O | ASP | A | 269 | 17.829 | 19.729 | 17.551 | 1.00 | 18.28 | O |
| ATOM | 2068 | CB | ASP | A | 269 | 16.069 | 21.436 | 15.532 | 1.00 | 20.34 | C |
| ATOM | 2069 | CG | ASP | A | 269 | 14.976 | 21.636 | 14.500 | 1.00 | 20.66 | C |
| ATOM | 2070 | OD1 | ASP | A | 269 | 14.977 | 21.015 | 13.419 | 1.00 | 22.15 | O |
| ATOM | 2071 | OD2 | ASP | A | 269 | 14.072 | 22.454 | 14.703 | 1.00 | 23.30 | O |
| ATOM | 2072 | N | VAL | A | 270 | 19.129 | 20.681 | 15.953 | 1.00 | 19.76 | N |
| ATOM | 2073 | CA | VAL | A | 270 | 20.304 | 20.879 | 16.782 | 1.00 | 20.24 | C |
| ATOM | 2074 | C | VAL | A | 270 | 20.793 | 22.318 | 16.601 | 1.00 | 19.84 | C |
| ATOM | 2075 | O | VAL | A | 270 | 21.052 | 22.754 | 15.487 | 1.00 | 19.90 | O |
| ATOM | 2076 | CB | VAL | A | 270 | 21.421 | 19.942 | 16.377 | 1.00 | 20.08 | C |
| ATOM | 2077 | CG1 | VAL | A | 270 | 22.676 | 20.288 | 17.121 | 1.00 | 21.38 | C |
| ATOM | 2078 | CG2 | VAL | A | 270 | 21.017 | 18.521 | 16.671 | 1.00 | 21.15 | C |
| ATOM | 2079 | N | LEU | A | 271 | 20.885 | 23.056 | 17.699 | 1.00 | 19.86 | N |
| ATOM | 2080 | CA | LEU | A | 271 | 21.341 | 24.427 | 17.656 | 1.00 | 20.03 | C |
| ATOM | 2081 | C | LEU | A | 271 | 22.757 | 24.465 | 18.202 | 1.00 | 20.23 | C |
| ATOM | 2082 | O | LEU | A | 271 | 23.032 | 23.946 | 19.276 | 1.00 | 19.73 | O |
| ATOM | 2083 | CB | LEU | A | 271 | 20.429 | 25.328 | 18.465 | 1.00 | 20.59 | C |
| ATOM | 2084 | CG | LEU | A | 271 | 20.934 | 26.742 | 18.724 | 1.00 | 20.93 | C |
| ATOM | 2085 | CD1 | LEU | A | 271 | 21.011 | 27.562 | 17.431 | 1.00 | 20.35 | C |
| ATOM | 2086 | CD2 | LEU | A | 271 | 20.039 | 27.428 | 19.728 | 1.00 | 22.31 | C |
| ATOM | 2087 | N | TYR | A | 272 | 23.669 | 25.024 | 17.416 | 1.00 | 20.58 | N |
| ATOM | 2088 | CA | TYR | A | 272 | 25.010 | 25.229 | 17.883 | 1.00 | 20.58 | C |
| ATOM | 2089 | C | TYR | A | 272 | 24.985 | 26.535 | 18.653 | 1.00 | 20.69 | C |
| ATOM | 2090 | O | TYR | A | 272 | 24.692 | 27.576 | 18.089 | 1.00 | 21.54 | O |
| ATOM | 2091 | CB | TYR | A | 272 | 26.004 | 25.312 | 16.728 | 1.00 | 20.30 | C |
| ATOM | 2092 | CG | TYR | A | 272 | 27.381 | 25.776 | 17.158 | 1.00 | 21.24 | C |
| ATOM | 2093 | CD1 | TYR | A | 272 | 27.997 | 25.250 | 18.275 | 1.00 | 21.70 | C |
| ATOM | 2094 | CD2 | TYR | A | 272 | 28.039 | 26.788 | 16.472 | 1.00 | 22.21 | C |
| ATOM | 2095 | CE1 | TYR | A | 272 | 29.232 | 25.692 | 18.674 | 1.00 | 21.69 | C |
| ATOM | 2096 | CE2 | TYR | A | 272 | 29.275 | 27.215 | 16.857 | 1.00 | 22.99 | C |
| ATOM | 2097 | CZ | TYR | A | 272 | 29.868 | 26.672 | 17.961 | 1.00 | 22.01 | C |
| ATOM | 2098 | OH | TYR | A | 272 | 31.109 | 27.111 | 18.352 | 1.00 | 22.77 | O |
| ATOM | 2099 | N | ILE | A | 273 | 25.216 | 26.454 | 19.951 | 1.00 | 21.22 | N |
| ATOM | 2100 | CA | ILE | A | 273 | 25.362 | 27.629 | 20.805 | 1.00 | 21.49 | C |
| ATOM | 2101 | C | ILE | A | 273 | 26.852 | 27.809 | 21.117 | 1.00 | 22.00 | C |
| ATOM | 2102 | O | ILE | A | 273 | 27.413 | 27.112 | 21.962 | 1.00 | 22.55 | O |
| ATOM | 2103 | CB | ILE | A | 273 | 24.607 | 27.471 | 22.073 | 1.00 | 21.14 | C |
| ATOM | 2104 | CG1 | ILE | A | 273 | 23.148 | 27.132 | 21.776 | 1.00 | 21.68 | C |
| ATOM | 2105 | CG2 | ILE | A | 273 | 24.661 | 28.791 | 22.854 | 1.00 | 21.75 | C |
| ATOM | 2106 | CD1 | ILE | A | 273 | 22.318 | 26.972 | 23.026 | 1.00 | 21.44 | C |
| ATOM | 2107 | N | PRO | A | 274 | 27.493 | 28.723 | 20.413 | 1.00 | 21.86 | N |
| ATOM | 2108 | CA | PRO | A | 274 | 28.929 | 28.916 | 20.557 | 1.00 | 22.49 | C |
| ATOM | 2109 | C | PRO | A | 274 | 29.278 | 29.462 | 21.926 | 1.00 | 22.77 | C |
| ATOM | 2110 | O | PRO | A | 274 | 28.510 | 30.231 | 22.521 | 1.00 | 21.72 | O |
| ATOM | 2111 | CB | PRO | A | 274 | 29.305 | 29.908 | 19.429 | 1.00 | 23.00 | C |
| ATOM | 2112 | CG | PRO | A | 274 | 28.022 | 30.225 | 18.658 | 1.00 | 23.03 | C |
| ATOM | 2113 | CD | PRO | A | 274 | 26.889 | 29.582 | 19.398 | 1.00 | 22.21 | C |
| ATOM | 2114 | N | MET | A | 275 | 30.441 | 29.028 | 22.404 | 1.00 | 22.72 | N |
| ATOM | 2115 | CA | MET | A | 275 | 30.962 | 29.403 | 23.702 | 1.00 | 23.40 | C |
| ATOM | 2116 | C | MET | A | 275 | 30.949 | 30.921 | 23.864 | 1.00 | 22.42 | C |
| ATOM | 2117 | O | MET | A | 275 | 31.282 | 31.636 | 22.937 | 1.00 | 20.73 | O |
| ATOM | 2118 | CB | MET | A | 275 | 32.373 | 28.856 | 23.826 | 1.00 | 23.99 | C |
| ATOM | 2119 | CG | MET | A | 275 | 32.933 | 28.944 | 25.203 | 1.00 | 28.99 | C |
| ATOM | 2120 | SD | MET | A | 275 | 34.517 | 28.083 | 25.337 | 1.00 | 35.05 | S |
| ATOM | 2121 | CE | MET | A | 275 | 35.287 | 28.525 | 23.832 | 1.00 | 31.30 | C |
| ATOM | 2122 | N | TYR | A | 276 | 30.509 | 31.388 | 25.030 | 1.00 | 22.30 | N |
| ATOM | 2123 | CA | TYR | A | 276 | 30.419 | 32.831 | 25.349 | 1.00 | 23.06 | C |
| ATOM | 2124 | C | TYR | A | 276 | 29.221 | 33.543 | 24.752 | 1.00 | 22.11 | C |
| ATOM | 2125 | O | TYR | A | 276 | 29.012 | 34.705 | 25.041 | 1.00 | 21.84 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2126 | CB | TYR | A | 276 | 31.673 | 33.594 | 24.934 | 1.00 | 23.42 | C |
| ATOM | 2127 | CG | TYR | A | 276 | 32.857 | 33.283 | 25.796 | 1.00 | 28.51 | C |
| ATOM | 2128 | CD1 | TYR | A | 276 | 32.969 | 33.799 | 27.072 | 1.00 | 33.00 | C |
| ATOM | 2129 | CD2 | TYR | A | 276 | 33.876 | 32.460 | 25.321 | 1.00 | 34.41 | C |
| ATOM | 2130 | CE1 | TYR | A | 276 | 34.066 | 33.490 | 27.877 | 1.00 | 36.36 | C |
| ATOM | 2131 | CE2 | TYR | A | 276 | 34.968 | 32.151 | 26.102 | 1.00 | 36.45 | C |
| ATOM | 2132 | CZ | TYR | A | 276 | 35.059 | 32.651 | 27.371 | 1.00 | 37.63 | C |
| ATOM | 2133 | OH | TYR | A | 276 | 36.192 | 32.314 | 28.077 | 1.00 | 40.88 | O |
| ATOM | 2134 | N | TRP | A | 277 | 28.455 | 32.878 | 23.906 | 1.00 | 20.75 | N |
| ATOM | 2135 | CA | TRP | A | 277 | 27.272 | 33.528 | 23.360 | 1.00 | 20.85 | C |
| ATOM | 2136 | C | TRP | A | 277 | 26.173 | 33.482 | 24.372 | 1.00 | 20.33 | C |
| ATOM | 2137 | O | TRP | A | 277 | 25.907 | 32.431 | 24.949 | 1.00 | 20.72 | O |
| ATOM | 2138 | CB | TRP | A | 277 | 26.791 | 32.874 | 22.068 | 1.00 | 20.13 | C |
| ATOM | 2139 | CG | TRP | A | 277 | 27.552 | 33.323 | 20.879 | 1.00 | 19.28 | C |
| ATOM | 2140 | CD1 | TRP | A | 277 | 28.887 | 33.175 | 20.673 | 1.00 | 21.27 | C |
| ATOM | 2141 | CD2 | TRP | A | 277 | 27.042 | 33.995 | 19.730 | 1.00 | 20.60 | C |
| ATOM | 2142 | NE1 | TRP | A | 277 | 29.246 | 33.721 | 19.467 | 1.00 | 21.05 | N |
| ATOM | 2143 | CE2 | TRP | A | 277 | 28.128 | 34.232 | 18.864 | 1.00 | 21.04 | C |
| ATOM | 2144 | CE3 | TRP | A | 277 | 25.780 | 34.456 | 19.352 | 1.00 | 21.08 | C |
| ATOM | 2145 | CZ2 | TRP | A | 277 | 27.989 | 34.893 | 17.643 | 1.00 | 20.38 | C |
| ATOM | 2146 | CZ3 | TRP | A | 277 | 25.641 | 35.110 | 18.122 | 1.00 | 20.48 | C |
| ATOM | 2147 | CH2 | TRP | A | 277 | 26.736 | 35.306 | 17.288 | 1.00 | 21.03 | C |
| ATOM | 2148 | N | TRP | A | 278 | 25.572 | 34.632 | 24.629 | 1.00 | 19.39 | N |
| ATOM | 2149 | CA | TRP | A | 278 | 24.430 | 34.711 | 25.521 | 1.00 | 19.80 | C |
| ATOM | 2150 | C | TRP | A | 278 | 23.243 | 33.927 | 24.927 | 1.00 | 20.18 | C |
| ATOM | 2151 | O | TRP | A | 278 | 23.019 | 33.939 | 23.732 | 1.00 | 21.04 | O |
| ATOM | 2152 | CB | TRP | A | 278 | 23.989 | 36.168 | 25.646 | 1.00 | 20.39 | C |
| ATOM | 2153 | CG | TRP | A | 278 | 24.979 | 37.031 | 26.300 | 1.00 | 21.20 | C |
| ATOM | 2154 | CD1 | TRP | A | 278 | 26.022 | 37.672 | 25.720 | 1.00 | 21.06 | C |
| ATOM | 2155 | CD2 | TRP | A | 278 | 25.056 | 37.301 | 27.691 | 1.00 | 20.38 | C |
| ATOM | 2156 | NE1 | TRP | A | 278 | 26.725 | 38.369 | 26.668 | 1.00 | 22.44 | N |
| ATOM | 2157 | CE2 | TRP | A | 278 | 26.139 | 38.155 | 27.891 | 1.00 | 21.86 | C |
| ATOM | 2158 | CE3 | TRP | A | 278 | 24.282 | 36.937 | 28.789 | 1.00 | 21.09 | C |
| ATOM | 2159 | CZ2 | TRP | A | 278 | 26.480 | 38.640 | 29.147 | 1.00 | 21.13 | C |
| ATOM | 2160 | CZ3 | TRP | A | 278 | 24.623 | 37.412 | 30.019 | 1.00 | 23.38 | C |
| ATOM | 2161 | CH2 | TRP | A | 278 | 25.704 | 38.258 | 30.194 | 1.00 | 21.06 | C |
| ATOM | 2162 | N | HIS | A | 279 | 22.465 | 33.278 | 25.761 | 1.00 | 20.76 | N |
| ATOM | 2163 | CA | HIS | A | 279 | 21.262 | 32.646 | 25.294 | 1.00 | 21.56 | C |
| ATOM | 2164 | C | HIS | A | 279 | 20.198 | 32.659 | 26.361 | 1.00 | 21.24 | C |
| ATOM | 2165 | O | HIS | A | 279 | 20.475 | 32.456 | 27.540 | 1.00 | 21.63 | O |
| ATOM | 2166 | CB | HIS | A | 279 | 21.501 | 31.203 | 24.819 | 1.00 | 21.83 | C |
| ATOM | 2167 | CG | HIS | A | 279 | 22.342 | 30.379 | 25.738 | 1.00 | 23.50 | C |
| ATOM | 2168 | ND1 | HIS | A | 279 | 23.713 | 30.494 | 25.785 | 1.00 | 24.98 | N |
| ATOM | 2169 | CD2 | HIS | A | 279 | 22.017 | 29.385 | 26.602 | 1.00 | 26.21 | C |
| ATOM | 2170 | CE1 | HIS | A | 279 | 24.200 | 29.599 | 26.628 | 1.00 | 26.46 | C |
| ATOM | 2171 | NE2 | HIS | A | 279 | 23.192 | 28.927 | 27.158 | 1.00 | 25.14 | N |
| ATOM | 2172 | N | HIS | A | 280 | 18.994 | 32.900 | 25.874 | 1.00 | 21.71 | N |
| ATOM | 2173 | CA | HIS | A | 280 | 17.736 | 32.956 | 26.602 | 1.00 | 21.78 | C |
| ATOM | 2174 | C | HIS | A | 280 | 16.890 | 31.860 | 25.951 | 1.00 | 21.70 | C |
| ATOM | 2175 | O | HIS | A | 280 | 16.722 | 31.846 | 24.736 | 1.00 | 21.40 | O |
| ATOM | 2176 | CB | HIS | A | 280 | 17.104 | 34.322 | 26.374 | 1.00 | 21.20 | C |
| ATOM | 2177 | CG | HIS | A | 280 | 15.642 | 34.367 | 26.626 | 1.00 | 21.64 | C |
| ATOM | 2178 | ND1 | HIS | A | 280 | 15.100 | 35.028 | 27.705 | 1.00 | 22.67 | N |
| ATOM | 2179 | CD2 | HIS | A | 280 | 14.600 | 33.826 | 25.951 | 1.00 | 23.33 | C |
| ATOM | 2180 | CE1 | HIS | A | 280 | 13.786 | 34.891 | 27.684 | 1.00 | 23.20 | C |
| ATOM | 2181 | NE2 | HIS | A | 280 | 13.457 | 34.158 | 26.635 | 1.00 | 23.30 | N |
| ATOM | 2182 | N | ILE | A | 281 | 16.368 | 30.934 | 26.733 | 1.00 | 22.98 | N |
| ATOM | 2183 | CA | ILE | A | 281 | 15.658 | 29.779 | 26.158 | 1.00 | 23.36 | C |
| ATOM | 2184 | C | ILE | A | 281 | 14.313 | 29.606 | 26.800 | 1.00 | 23.58 | C |
| ATOM | 2185 | O | ILE | A | 281 | 14.209 | 29.592 | 28.014 | 1.00 | 23.63 | O |
| ATOM | 2186 | CB | ILE | A | 281 | 16.512 | 28.525 | 26.301 | 1.00 | 23.87 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2187 | CG1 | ILE | A | 281 | 17.771 | 28.675 | 25.435 | 1.00 | 25.77 | C |
| ATOM | 2188 | CG2 | ILE | A | 281 | 15.748 | 27.261 | 25.863 | 1.00 | 23.54 | C |
| ATOM | 2189 | CD1 | ILE | A | 281 | 18.752 | 27.659 | 25.690 | 1.00 | 29.36 | C |
| ATOM | 2190 | N | GLU | A | 282 | 13.268 | 29.510 | 25.982 | 1.00 | 23.92 | N |
| ATOM | 2191 | CA | GLU | A | 282 | 11.923 | 29.337 | 26.525 | 1.00 | 24.26 | C |
| ATOM | 2192 | C | GLU | A | 282 | 11.113 | 28.234 | 25.834 | 1.00 | 23.82 | C |
| ATOM | 2193 | O | GLU | A | 282 | 11.115 | 28.107 | 24.606 | 1.00 | 24.00 | O |
| ATOM | 2194 | CB | GLU | A | 282 | 11.166 | 30.681 | 26.490 | 1.00 | 24.35 | C |
| ATOM | 2195 | CG | GLU | A | 282 | 10.887 | 31.249 | 25.112 | 1.00 | 25.59 | C |
| ATOM | 2196 | CD | GLU | A | 282 | 10.320 | 32.668 | 25.168 | 1.00 | 25.45 | C |
| ATOM | 2197 | OE1 | GLU | A | 282 | 10.861 | 33.494 | 25.929 | 1.00 | 26.04 | O |
| ATOM | 2198 | OE2 | GLU | A | 282 | 9.332 | 32.954 | 24.451 | 1.00 | 25.08 | O |
| ATOM | 2199 | N | SER | A | 283 | 10.460 | 27.419 | 26.648 | 1.00 | 23.28 | N |
| ATOM | 2200 | CA | SER | A | 283 | 9.573 | 26.373 | 26.166 | 1.00 | 23.66 | C |
| ATOM | 2201 | C | SER | A | 283 | 8.257 | 27.054 | 25.787 | 1.00 | 23.86 | C |
| ATOM | 2202 | O | SER | A | 283 | 7.678 | 27.780 | 26.593 | 1.00 | 23.20 | O |
| ATOM | 2203 | CB | SER | A | 283 | 9.341 | 25.321 | 27.247 | 1.00 | 23.36 | C |
| ATOM | 2204 | OG | SER | A | 283 | 10.473 | 24.497 | 27.401 | 1.00 | 23.30 | O |
| ATOM | 2205 | N | LEU | A | 284 | 7.792 | 26.837 | 24.564 | 1.00 | 24.56 | N |
| ATOM | 2206 | CA | LEU | A | 284 | 6.626 | 27.583 | 24.084 | 1.00 | 25.62 | C |
| ATOM | 2207 | C | LEU | A | 284 | 5.401 | 27.487 | 25.004 | 1.00 | 25.52 | C |
| ATOM | 2208 | O | LEU | A | 284 | 5.114 | 26.431 | 25.589 | 1.00 | 24.71 | O |
| ATOM | 2209 | CB | LEU | A | 284 | 6.237 | 27.157 | 22.680 | 1.00 | 25.64 | C |
| ATOM | 2210 | CG | LEU | A | 284 | 7.274 | 27.308 | 21.576 | 1.00 | 27.12 | C |
| ATOM | 2211 | CD1 | LEU | A | 284 | 6.591 | 27.546 | 20.242 | 1.00 | 28.93 | C |
| ATOM | 2212 | CD2 | LEU | A | 284 | 8.248 | 28.364 | 21.851 | 1.00 | 27.08 | C |
| ATOM | 2213 | N | LEU | A | 285 | 4.713 | 28.615 | 25.144 | 1.00 | 25.85 | N |
| ATOM | 2214 | CA | LEU | A | 285 | 3.490 | 28.676 | 25.942 | 1.00 | 26.84 | C |
| ATOM | 2215 | C | LEU | A | 285 | 2.507 | 27.691 | 25.345 | 1.00 | 27.10 | C |
| ATOM | 2216 | O | LEU | A | 285 | 2.424 | 27.565 | 24.139 | 1.00 | 27.10 | O |
| ATOM | 2217 | CB | LEU | A | 285 | 2.875 | 30.071 | 25.906 | 1.00 | 26.48 | C |
| ATOM | 2218 | CG | LEU | A | 285 | 3.709 | 31.225 | 26.438 | 1.00 | 27.70 | C |
| ATOM | 2219 | CD1 | LEU | A | 285 | 3.075 | 32.554 | 26.026 | 1.00 | 28.22 | C |
| ATOM | 2220 | CD2 | LEU | A | 285 | 3.845 | 31.125 | 27.928 | 1.00 | 28.39 | C |
| ATOM | 2221 | N | ASN | A | 286 | 1.779 | 26.987 | 26.196 | 1.00 | 27.81 | N |
| ATOM | 2222 | CA | ASN | A | 286 | 0.790 | 26.007 | 25.753 | 1.00 | 28.27 | C |
| ATOM | 2223 | C | ASN | A | 286 | 1.313 | 24.977 | 24.744 | 1.00 | 27.42 | C |
| ATOM | 2224 | O | ASN | A | 286 | 0.555 | 24.481 | 23.922 | 1.00 | 26.50 | O |
| ATOM | 2225 | CB | ASN | A | 286 | -0.417 | 26.741 | 25.160 | 1.00 | 29.08 | C |
| ATOM | 2226 | CG | ASN | A | 286 | -0.931 | 27.846 | 26.078 | 1.00 | 32.15 | C |
| ATOM | 2227 | OD1 | ASN | A | 286 | -1.484 | 27.577 | 27.154 | 1.00 | 34.93 | O |
| ATOM | 2228 | ND2 | ASN | A | 286 | -0.725 | 29.099 | 25.670 | 1.00 | 35.91 | N |
| ATOM | 2229 | N | GLY | A | 287 | 2.608 | 24.672 | 24.799 | 1.00 | 26.54 | N |
| ATOM | 2230 | CA | GLY | A | 287 | 3.201 | 23.727 | 23.879 | 1.00 | 25.64 | C |
| ATOM | 2231 | C | GLY | A | 287 | 3.474 | 22.371 | 24.497 | 1.00 | 25.01 | C |
| ATOM | 2232 | O | GLY | A | 287 | 4.031 | 21.502 | 23.829 | 1.00 | 24.77 | O |
| ATOM | 2233 | N | GLY | A | 288 | 3.110 | 22.187 | 25.766 | 1.00 | 24.43 | N |
| ATOM | 2234 | CA | GLY | A | 288 | 3.357 | 20.922 | 26.455 | 1.00 | 23.99 | C |
| ATOM | 2235 | C | GLY | A | 288 | 4.804 | 20.844 | 26.935 | 1.00 | 24.11 | C |
| ATOM | 2236 | O | GLY | A | 288 | 5.546 | 21.810 | 26.786 | 1.00 | 22.82 | O |
| ATOM | 2237 | N | ILE | A | 289 | 5.211 | 19.695 | 27.472 | 1.00 | 23.99 | N |
| ATOM | 2238 | CA | ILE | A | 289 | 6.550 | 19.522 | 28.000 | 1.00 | 24.69 | C |
| ATOM | 2239 | C | ILE | A | 289 | 7.605 | 19.496 | 26.908 | 1.00 | 24.25 | C |
| ATOM | 2240 | O | ILE | A | 289 | 7.350 | 19.092 | 25.774 | 1.00 | 25.20 | O |
| ATOM | 2241 | CB | ILE | A | 289 | 6.691 | 18.234 | 28.836 | 1.00 | 25.39 | C |
| ATOM | 2242 | CG1 | ILE | A | 289 | 6.702 | 17.006 | 27.941 | 1.00 | 27.43 | C |
| ATOM | 2243 | CG2 | ILE | A | 289 | 5.613 | 18.151 | 29.921 | 1.00 | 26.30 | C |
| ATOM | 2244 | CD1 | ILE | A | 289 | 7.255 | 15.752 | 28.650 | 1.00 | 30.57 | C |
| ATOM | 2245 | N | THR | A | 290 | 8.808 | 19.912 | 27.267 | 1.00 | 23.28 | N |
| ATOM | 2246 | CA | THR | A | 290 | 9.908 | 19.908 | 26.334 | 1.00 | 22.12 | C |
| ATOM | 2247 | C | THR | A | 290 | 11.008 | 18.984 | 26.824 | 1.00 | 21.52 | C |

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ATOM   2248  O   THR A 290      11.193  18.789  28.029  1.00 20.85           O
ATOM   2249  CB  THR A 290      10.473  21.318  26.168  1.00 22.19           C
ATOM   2250  OG1 THR A 290      10.758  21.885  27.444  1.00 21.69           O
ATOM   2251  CG2 THR A 290       9.436  22.268  25.557  1.00 23.05           C
ATOM   2252  N   ILE A 291      11.746  18.421  25.880  1.00 20.44           N
ATOM   2253  CA  ILE A 291      12.880  17.616  26.234  1.00 21.24           C
ATOM   2254  C   ILE A 291      14.033  17.981  25.347  1.00 20.47           C
ATOM   2255  O   ILE A 291      13.869  18.064  24.137  1.00 21.04           O
ATOM   2256  CB  ILE A 291      12.559  16.118  26.078  1.00 21.40           C
ATOM   2257  CG1 ILE A 291      11.405  15.724  27.004  1.00 22.31           C
ATOM   2258  CG2 ILE A 291      13.798  15.310  26.383  1.00 22.63           C
ATOM   2259  CD1 ILE A 291      10.969  14.262  26.867  1.00 23.92           C
ATOM   2260  N   THR A 292      15.194  18.188  25.953  1.00 20.24           N
ATOM   2261  CA  THR A 292      16.395  18.517  25.236  1.00 20.13           C
ATOM   2262  C   THR A 292      17.560  17.794  25.831  1.00 20.29           C
ATOM   2263  O   THR A 292      17.605  17.557  27.021  1.00 20.94           O
ATOM   2264  CB  THR A 292      16.688  20.044  25.365  1.00 20.34           C
ATOM   2265  OG1 THR A 292      15.524  20.799  25.022  1.00 19.08           O
ATOM   2266  CG2 THR A 292      17.730  20.487  24.355  1.00 20.32           C
ATOM   2267  N   VAL A 293      18.530  17.454  25.003  1.00 20.52           N
ATOM   2268  CA  VAL A 293      19.784  16.939  25.516  1.00 20.48           C
ATOM   2269  C   VAL A 293      20.892  17.803  24.918  1.00 20.80           C
ATOM   2270  O   VAL A 293      20.936  17.954  23.709  1.00 19.58           O
ATOM   2271  CB  VAL A 293      19.995  15.483  25.129  1.00 20.78           C
ATOM   2272  CG1 VAL A 293      21.436  15.068  25.385  1.00 20.33           C
ATOM   2273  CG2 VAL A 293      19.047  14.597  25.919  1.00 20.95           C
ATOM   2274  N   ASN A 294      21.749  18.412  25.752  1.00 21.34           N
ATOM   2275  CA  ASN A 294      22.855  19.192  25.205  1.00 22.04           C
ATOM   2276  C   ASN A 294      24.144  18.362  25.204  1.00 22.29           C
ATOM   2277  O   ASN A 294      24.182  17.241  25.720  1.00 23.22           O
ATOM   2278  CB  ASN A 294      23.012  20.581  25.883  1.00 22.35           C
ATOM   2279  CG  ASN A 294      23.703  20.520  27.259  1.00 23.08           C
ATOM   2280  OD1 ASN A 294      24.240  19.493  27.628  1.00 22.91           O
ATOM   2281  ND2 ASN A 294      23.657  21.640  28.027  1.00 21.75           N
ATOM   2282  N   PHE A 295      25.168  18.903  24.565  1.00 22.27           N
ATOM   2283  CA  PHE A 295      26.467  18.269  24.452  1.00 22.31           C
ATOM   2284  C   PHE A 295      27.444  19.408  24.704  1.00 22.66           C
ATOM   2285  O   PHE A 295      27.602  20.299  23.865  1.00 23.12           O
ATOM   2286  CB  PHE A 295      26.709  17.748  23.040  1.00 22.32           C
ATOM   2287  CG  PHE A 295      25.871  16.568  22.653  1.00 22.18           C
ATOM   2288  CD1 PHE A 295      24.494  16.689  22.477  1.00 22.38           C
ATOM   2289  CD2 PHE A 295      26.465  15.336  22.441  1.00 21.44           C
ATOM   2290  CE1 PHE A 295      23.757  15.604  22.111  1.00 24.06           C
ATOM   2291  CE2 PHE A 295      25.718  14.248  22.064  1.00 19.77           C
ATOM   2292  CZ  PHE A 295      24.380  14.366  21.911  1.00 21.39           C
ATOM   2293  N   TRP A 296      28.062  19.403  25.869  1.00 22.66           N
ATOM   2294  CA  TRP A 296      28.998  20.450  26.256  1.00 23.09           C
ATOM   2295  C   TRP A 296      30.454  19.991  26.081  1.00 23.22           C
ATOM   2296  O   TRP A 296      30.865  18.932  26.595  1.00 22.78           O
ATOM   2297  CB  TRP A 296      28.734  20.834  27.707  1.00 22.89           C
ATOM   2298  CG  TRP A 296      27.830  22.013  27.906  1.00 23.61           C
ATOM   2299  CD1 TRP A 296      27.783  23.129  27.149  1.00 25.47           C
ATOM   2300  CD2 TRP A 296      26.894  22.219  28.975  1.00 24.55           C
ATOM   2301  NE1 TRP A 296      26.874  24.018  27.667  1.00 25.25           N
ATOM   2302  CE2 TRP A 296      26.308  23.478  28.783  1.00 24.33           C
ATOM   2303  CE3 TRP A 296      26.464  21.444  30.061  1.00 27.49           C
ATOM   2304  CZ2 TRP A 296      25.335  23.994  29.631  1.00 25.91           C
ATOM   2305  CZ3 TRP A 296      25.474  21.952  30.899  1.00 27.19           C
ATOM   2306  CH2 TRP A 296      24.935  23.224  30.682  1.00 26.96           C
ATOM   2307  N   TYR A 297      31.216  20.783  25.337  1.00 23.29           N
ATOM   2308  CA  TYR A 297      32.627  20.510  25.100  1.00 23.80           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2309 | C | TYR | A | 297 | 33.506 | 21.660 | 25.554 | 1.00 | 24.51 | C |
| ATOM | 2310 | O | TYR | A | 297 | 33.188 | 22.825 | 25.323 | 1.00 | 23.73 | O |
| ATOM | 2311 | CB | TYR | A | 297 | 32.882 | 20.332 | 23.610 | 1.00 | 23.38 | C |
| ATOM | 2312 | CG | TYR | A | 297 | 32.284 | 19.092 | 23.021 | 1.00 | 23.42 | C |
| ATOM | 2313 | CD1 | TYR | A | 297 | 30.940 | 19.053 | 22.641 | 1.00 | 23.90 | C |
| ATOM | 2314 | CD2 | TYR | A | 297 | 33.056 | 17.971 | 22.808 | 1.00 | 21.43 | C |
| ATOM | 2315 | CE1 | TYR | A | 297 | 30.394 | 17.920 | 22.089 | 1.00 | 23.32 | C |
| ATOM | 2316 | CE2 | TYR | A | 297 | 32.515 | 16.826 | 22.250 | 1.00 | 22.05 | C |
| ATOM | 2317 | CZ | TYR | A | 297 | 31.186 | 16.806 | 21.905 | 1.00 | 21.88 | C |
| ATOM | 2318 | OH | TYR | A | 297 | 30.644 | 15.669 | 21.365 | 1.00 | 21.30 | O |
| ATOM | 2319 | N | LYS | A | 298 | 34.637 | 21.334 | 26.160 | 1.00 | 25.35 | N |
| ATOM | 2320 | CA | LYS | A | 298 | 35.589 | 22.362 | 26.536 | 1.00 | 26.48 | C |
| ATOM | 2321 | C | LYS | A | 298 | 36.070 | 23.017 | 25.268 | 1.00 | 26.23 | C |
| ATOM | 2322 | O | LYS | A | 298 | 36.224 | 22.364 | 24.249 | 1.00 | 24.85 | O |
| ATOM | 2323 | CB | LYS | A | 298 | 36.783 | 21.771 | 27.308 | 1.00 | 27.15 | C |
| ATOM | 2324 | CG | LYS | A | 298 | 36.474 | 21.471 | 28.777 | 1.00 | 30.00 | C |
| ATOM | 2325 | CD | LYS | A | 298 | 37.666 | 20.901 | 29.550 | 1.00 | 33.20 | C |
| ATOM | 2326 | CE | LYS | A | 298 | 37.232 | 20.493 | 30.969 | 1.00 | 36.09 | C |
| ATOM | 2327 | NZ | LYS | A | 298 | 38.299 | 19.766 | 31.764 | 1.00 | 39.03 | N |
| ATOM | 2328 | N | GLY | A | 299 | 36.321 | 24.313 | 25.329 | 1.00 | 27.13 | N |
| ATOM | 2329 | CA | GLY | A | 299 | 36.798 | 25.014 | 24.159 | 1.00 | 28.27 | C |
| ATOM | 2330 | C | GLY | A | 299 | 38.229 | 24.649 | 23.837 | 1.00 | 29.23 | C |
| ATOM | 2331 | O | GLY | A | 299 | 38.892 | 24.005 | 24.613 | 1.00 | 28.19 | O |
| ATOM | 2332 | N | ALA | A | 300 | 38.674 | 25.046 | 22.660 | 1.00 | 31.78 | N |
| ATOM | 2333 | CA | ALA | A | 300 | 40.046 | 24.852 | 22.233 | 1.00 | 34.32 | C |
| ATOM | 2334 | C | ALA | A | 300 | 40.992 | 25.610 | 23.155 | 1.00 | 36.37 | C |
| ATOM | 2335 | O | ALA | A | 300 | 40.573 | 26.430 | 23.956 | 1.00 | 35.96 | O |
| ATOM | 2336 | CB | ALA | A | 300 | 40.210 | 25.355 | 20.806 | 1.00 | 34.38 | C |
| ATOM | 2337 | N | PRO | A | 301 | 42.280 | 25.349 | 23.025 | 1.00 | 39.70 | N |
| ATOM | 2338 | CA | PRO | A | 301 | 43.278 | 26.051 | 23.845 | 1.00 | 41.64 | C |
| ATOM | 2339 | C | PRO | A | 301 | 43.465 | 27.482 | 23.386 | 1.00 | 43.35 | C |
| ATOM | 2340 | O | PRO | A | 301 | 43.220 | 27.803 | 22.228 | 1.00 | 43.86 | O |
| ATOM | 2341 | CB | PRO | A | 301 | 44.566 | 25.275 | 23.572 | 1.00 | 41.46 | C |
| ATOM | 2342 | CG | PRO | A | 301 | 44.382 | 24.736 | 22.199 | 1.00 | 41.25 | C |
| ATOM | 2343 | CD | PRO | A | 301 | 42.906 | 24.416 | 22.068 | 1.00 | 40.04 | C |
| ATOM | 2344 | N | THR | A | 302 | 43.900 | 28.328 | 24.300 | 1.00 | 45.97 | N |
| ATOM | 2345 | CA | THR | A | 302 | 44.214 | 29.715 | 24.001 | 1.00 | 47.77 | C |
| ATOM | 2346 | C | THR | A | 302 | 45.593 | 29.713 | 23.362 | 1.00 | 48.92 | C |
| ATOM | 2347 | O | THR | A | 302 | 46.532 | 29.251 | 24.006 | 1.00 | 49.23 | O |
| ATOM | 2348 | CB | THR | A | 302 | 44.282 | 30.469 | 25.322 | 1.00 | 48.10 | C |
| ATOM | 2349 | OG1 | THR | A | 302 | 43.006 | 30.416 | 25.976 | 1.00 | 49.37 | O |
| ATOM | 2350 | CG2 | THR | A | 302 | 44.520 | 31.924 | 25.100 | 1.00 | 48.91 | C |
| ATOM | 2351 | N | PRO | A | 303 | 45.761 | 30.248 | 22.148 | 1.00 | 50.22 | N |
| ATOM | 2352 | CA | PRO | A | 303 | 47.064 | 30.150 | 21.474 | 1.00 | 50.62 | C |
| ATOM | 2353 | C | PRO | A | 303 | 48.191 | 30.728 | 22.316 | 1.00 | 50.64 | C |
| ATOM | 2354 | O | PRO | A | 303 | 47.883 | 31.390 | 23.307 | 1.00 | 50.98 | O |
| ATOM | 2355 | CB | PRO | A | 303 | 46.877 | 30.986 | 20.202 | 1.00 | 50.93 | C |
| ATOM | 2356 | CG | PRO | A | 303 | 45.407 | 30.999 | 19.968 | 1.00 | 50.70 | C |
| ATOM | 2357 | CD | PRO | A | 303 | 44.814 | 31.064 | 21.360 | 1.00 | 50.45 | C |
| ATOM | 2358 | N | GLU | A | 307 | 46.978 | 37.074 | 18.830 | 1.00 | 53.59 | N |
| ATOM | 2359 | CA | GLU | A | 307 | 46.946 | 38.016 | 17.714 | 1.00 | 53.82 | C |
| ATOM | 2360 | C | GLU | A | 307 | 45.902 | 39.090 | 17.922 | 1.00 | 52.97 | C |
| ATOM | 2361 | O | GLU | A | 307 | 44.792 | 38.810 | 18.358 | 1.00 | 53.64 | O |
| ATOM | 2362 | CB | GLU | A | 307 | 46.672 | 37.308 | 16.371 | 1.00 | 54.37 | C |
| ATOM | 2363 | CG | GLU | A | 307 | 46.875 | 38.231 | 15.159 | 1.00 | 56.16 | C |
| ATOM | 2364 | CD | GLU | A | 307 | 46.966 | 37.504 | 13.822 | 1.00 | 57.96 | C |
| ATOM | 2365 | OE1 | GLU | A | 307 | 46.621 | 36.303 | 13.738 | 1.00 | 59.31 | O |
| ATOM | 2366 | OE2 | GLU | A | 307 | 47.388 | 38.150 | 12.839 | 1.00 | 59.69 | O |
| ATOM | 2367 | N | TYR | A | 308 | 46.267 | 40.324 | 17.610 | 1.00 | 51.95 | N |
| ATOM | 2368 | CA | TYR | A | 308 | 45.343 | 41.436 | 17.702 | 1.00 | 51.19 | C |
| ATOM | 2369 | C | TYR | A | 308 | 44.693 | 41.603 | 16.337 | 1.00 | 50.27 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2370 | O | TYR | A | 308 | 45.246 | 41.146 | 15.331 | 1.00 | 50.45 | O |
| ATOM | 2371 | CB | TYR | A | 308 | 46.083 | 42.684 | 18.162 | 1.00 | 51.43 | C |
| ATOM | 2372 | CG | TYR | A | 308 | 46.675 | 42.460 | 19.532 | 1.00 | 52.65 | C |
| ATOM | 2373 | CD1 | TYR | A | 308 | 45.925 | 42.712 | 20.674 | 1.00 | 52.95 | C |
| ATOM | 2374 | CD2 | TYR | A | 308 | 47.948 | 41.912 | 19.685 | 1.00 | 53.42 | C |
| ATOM | 2375 | CE1 | TYR | A | 308 | 46.435 | 42.472 | 21.925 | 1.00 | 54.01 | C |
| ATOM | 2376 | CE2 | TYR | A | 308 | 48.467 | 41.662 | 20.937 | 1.00 | 54.33 | C |
| ATOM | 2377 | CZ | TYR | A | 308 | 47.703 | 41.949 | 22.058 | 1.00 | 54.84 | C |
| ATOM | 2378 | OH | TYR | A | 308 | 48.189 | 41.714 | 23.323 | 1.00 | 56.45 | O |
| ATOM | 2379 | N | PRO | A | 309 | 43.496 | 42.186 | 16.290 | 1.00 | 48.69 | N |
| ATOM | 2380 | CA | PRO | A | 309 | 42.789 | 42.696 | 17.474 | 1.00 | 47.07 | C |
| ATOM | 2381 | C | PRO | A | 309 | 42.127 | 41.586 | 18.280 | 1.00 | 44.55 | C |
| ATOM | 2382 | O | PRO | A | 309 | 41.782 | 40.555 | 17.728 | 1.00 | 45.01 | O |
| ATOM | 2383 | CB | PRO | A | 309 | 41.720 | 43.606 | 16.869 | 1.00 | 47.45 | C |
| ATOM | 2384 | CG | PRO | A | 309 | 41.420 | 42.978 | 15.508 | 1.00 | 48.43 | C |
| ATOM | 2385 | CD | PRO | A | 309 | 42.701 | 42.336 | 15.056 | 1.00 | 48.78 | C |
| ATOM | 2386 | N | LEU | A | 310 | 41.967 | 41.790 | 19.577 | 1.00 | 41.78 | N |
| ATOM | 2387 | CA | LEU | A | 310 | 41.344 | 40.781 | 20.427 | 1.00 | 39.59 | C |
| ATOM | 2388 | C | LEU | A | 310 | 39.858 | 40.652 | 20.133 | 1.00 | 37.52 | C |
| ATOM | 2389 | O | LEU | A | 310 | 39.171 | 41.655 | 19.923 | 1.00 | 38.11 | O |
| ATOM | 2390 | CB | LEU | A | 310 | 41.499 | 41.174 | 21.893 | 1.00 | 39.43 | C |
| ATOM | 2391 | CG | LEU | A | 310 | 42.527 | 40.468 | 22.784 | 1.00 | 38.86 | C |
| ATOM | 2392 | CD1 | LEU | A | 310 | 43.799 | 40.123 | 22.092 | 1.00 | 37.07 | C |
| ATOM | 2393 | CD2 | LEU | A | 310 | 42.799 | 41.326 | 24.000 | 1.00 | 38.37 | C |
| ATOM | 2394 | N | LYS | A | 311 | 39.361 | 39.425 | 20.141 | 1.00 | 34.45 | N |
| ATOM | 2395 | CA | LYS | A | 311 | 37.932 | 39.180 | 20.001 | 1.00 | 32.51 | C |
| ATOM | 2396 | C | LYS | A | 311 | 37.144 | 39.537 | 21.257 | 1.00 | 30.59 | C |
| ATOM | 2397 | O | LYS | A | 311 | 37.675 | 39.546 | 22.375 | 1.00 | 28.88 | O |
| ATOM | 2398 | CB | LYS | A | 311 | 37.674 | 37.736 | 19.652 | 1.00 | 32.87 | C |
| ATOM | 2399 | N | ALA | A | 312 | 35.853 | 39.786 | 21.057 | 1.00 | 28.39 | N |
| ATOM | 2400 | CA | ALA | A | 312 | 34.991 | 40.141 | 22.155 | 1.00 | 27.14 | C |
| ATOM | 2401 | C | ALA | A | 312 | 35.110 | 39.121 | 23.260 | 1.00 | 26.12 | C |
| ATOM | 2402 | O | ALA | A | 312 | 35.274 | 39.509 | 24.411 | 1.00 | 24.47 | O |
| ATOM | 2403 | CB | ALA | A | 312 | 33.552 | 40.323 | 21.710 | 1.00 | 26.63 | C |
| ATOM | 2404 | N | HIS | A | 313 | 35.126 | 37.830 | 22.910 | 1.00 | 25.90 | N |
| ATOM | 2405 | CA | HIS | A | 313 | 35.106 | 36.796 | 23.932 | 1.00 | 25.82 | C |
| ATOM | 2406 | C | HIS | A | 313 | 36.411 | 36.749 | 24.690 | 1.00 | 25.03 | C |
| ATOM | 2407 | O | HIS | A | 313 | 36.447 | 36.323 | 25.825 | 1.00 | 24.89 | O |
| ATOM | 2408 | CB | HIS | A | 313 | 34.724 | 35.406 | 23.368 | 1.00 | 27.19 | C |
| ATOM | 2409 | CG | HIS | A | 313 | 35.788 | 34.773 | 22.535 | 1.00 | 29.47 | C |
| ATOM | 2410 | ND1 | HIS | A | 313 | 35.963 | 35.078 | 21.198 | 1.00 | 34.94 | N |
| ATOM | 2411 | CD2 | HIS | A | 313 | 36.753 | 33.880 | 22.847 | 1.00 | 33.69 | C |
| ATOM | 2412 | CE1 | HIS | A | 313 | 37.006 | 34.411 | 20.730 | 1.00 | 35.11 | C |
| ATOM | 2413 | NE2 | HIS | A | 313 | 37.495 | 33.665 | 21.705 | 1.00 | 35.57 | N |
| ATOM | 2414 | N | GLN | A | 314 | 37.491 | 37.185 | 24.072 | 1.00 | 24.60 | N |
| ATOM | 2415 | CA | GLN | A | 314 | 38.764 | 37.226 | 24.753 | 1.00 | 24.57 | C |
| ATOM | 2416 | C | GLN | A | 314 | 38.776 | 38.352 | 25.813 | 1.00 | 24.74 | C |
| ATOM | 2417 | O | GLN | A | 314 | 39.371 | 38.201 | 26.881 | 1.00 | 24.48 | O |
| ATOM | 2418 | CB | GLN | A | 314 | 39.898 | 37.420 | 23.745 | 1.00 | 24.79 | C |
| ATOM | 2419 | CG | GLN | A | 314 | 40.067 | 36.241 | 22.794 | 1.00 | 26.08 | C |
| ATOM | 2420 | CD | GLN | A | 314 | 41.109 | 36.488 | 21.730 | 1.00 | 27.10 | C |
| ATOM | 2421 | OE1 | GLN | A | 314 | 41.013 | 37.450 | 20.949 | 1.00 | 27.68 | O |
| ATOM | 2422 | NE2 | GLN | A | 314 | 42.123 | 35.629 | 21.699 | 1.00 | 29.52 | N |
| ATOM | 2423 | N | LYS | A | 315 | 38.115 | 39.462 | 25.506 | 1.00 | 23.99 | N |
| ATOM | 2424 | CA | LYS | A | 315 | 37.983 | 40.545 | 26.454 | 1.00 | 24.95 | C |
| ATOM | 2425 | C | LYS | A | 315 | 37.099 | 40.114 | 27.622 | 1.00 | 24.32 | C |
| ATOM | 2426 | O | LYS | A | 315 | 37.345 | 40.491 | 28.765 | 1.00 | 22.87 | O |
| ATOM | 2427 | CB | LYS | A | 315 | 37.408 | 41.783 | 25.785 | 1.00 | 25.11 | C |
| ATOM | 2428 | CG | LYS | A | 315 | 38.403 | 42.449 | 24.874 | 1.00 | 29.28 | C |
| ATOM | 2429 | CD | LYS | A | 315 | 37.821 | 43.693 | 24.226 | 1.00 | 34.17 | C |
| ATOM | 2430 | CE | LYS | A | 315 | 38.844 | 44.360 | 23.332 | 1.00 | 37.47 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2431 | NZ | LYS | A | 315 | 38.206 | 45.270 | 22.318 | 1.00 | 41.38 | N |
| ATOM | 2432 | N | VAL | A | 316 | 36.079 | 39.314 | 27.330 | 1.00 | 23.78 | N |
| ATOM | 2433 | CA | VAL | A | 316 | 35.258 | 38.796 | 28.396 | 1.00 | 23.67 | C |
| ATOM | 2434 | C | VAL | A | 316 | 36.138 | 37.937 | 29.329 | 1.00 | 23.61 | C |
| ATOM | 2435 | O | VAL | A | 316 | 36.094 | 38.075 | 30.558 | 1.00 | 22.63 | O |
| ATOM | 2436 | CB | VAL | A | 316 | 34.092 | 37.961 | 27.873 | 1.00 | 23.67 | C |
| ATOM | 2437 | CG1 | VAL | A | 316 | 33.315 | 37.370 | 29.037 | 1.00 | 23.53 | C |
| ATOM | 2438 | CG2 | VAL | A | 316 | 33.159 | 38.816 | 27.005 | 1.00 | 23.69 | C |
| ATOM | 2439 | N | ALA | A | 317 | 36.940 | 37.065 | 28.732 | 1.00 | 22.51 | N |
| ATOM | 2440 | CA | ALA | A | 317 | 37.834 | 36.207 | 29.507 | 1.00 | 22.28 | C |
| ATOM | 2441 | C | ALA | A | 317 | 38.730 | 37.067 | 30.391 | 1.00 | 21.32 | C |
| ATOM | 2442 | O | ALA | A | 317 | 38.926 | 36.783 | 31.556 | 1.00 | 21.45 | O |
| ATOM | 2443 | CB | ALA | A | 317 | 38.680 | 35.325 | 28.574 | 1.00 | 21.87 | C |
| ATOM | 2444 | N | ILE | A | 318 | 39.220 | 38.153 | 29.834 | 1.00 | 20.92 | N |
| ATOM | 2445 | CA | ILE | A | 318 | 40.091 | 39.053 | 30.574 | 1.00 | 21.36 | C |
| ATOM | 2446 | C | ILE | A | 318 | 39.375 | 39.662 | 31.784 | 1.00 | 21.54 | C |
| ATOM | 2447 | O | ILE | A | 318 | 39.930 | 39.697 | 32.895 | 1.00 | 20.69 | O |
| ATOM | 2448 | CB | ILE | A | 318 | 40.650 | 40.153 | 29.646 | 1.00 | 21.19 | C |
| ATOM | 2449 | CG1 | ILE | A | 318 | 41.664 | 39.560 | 28.670 | 1.00 | 21.41 | C |
| ATOM | 2450 | CG2 | ILE | A | 318 | 41.315 | 41.267 | 30.461 | 1.00 | 21.05 | C |
| ATOM | 2451 | CD1 | ILE | A | 318 | 42.217 | 40.569 | 27.663 | 1.00 | 21.73 | C |
| ATOM | 2452 | N | MET | A | 319 | 38.146 | 40.122 | 31.569 | 1.00 | 21.31 | N |
| ATOM | 2453 | CA | MET | A | 319 | 37.400 | 40.774 | 32.632 | 1.00 | 21.99 | C |
| ATOM | 2454 | C | MET | A | 319 | 37.094 | 39.787 | 33.748 | 1.00 | 22.21 | C |
| ATOM | 2455 | O | MET | A | 319 | 37.219 | 40.114 | 34.937 | 1.00 | 23.25 | O |
| ATOM | 2456 | CB | MET | A | 319 | 36.133 | 41.446 | 32.108 | 1.00 | 21.66 | C |
| ATOM | 2457 | CG | MET | A | 319 | 36.369 | 42.703 | 31.233 | 1.00 | 21.49 | C |
| ATOM | 2458 | SD | MET | A | 319 | 34.787 | 43.525 | 30.787 | 1.00 | 23.05 | S |
| ATOM | 2459 | CE | MET | A | 319 | 34.192 | 42.395 | 29.453 | 1.00 | 22.63 | C |
| ATOM | 2460 | N | ARG | A | 320 | 36.736 | 38.568 | 33.379 | 1.00 | 21.99 | N |
| ATOM | 2461 | CA | ARG | A | 320 | 36.492 | 37.544 | 34.383 | 1.00 | 21.57 | C |
| ATOM | 2462 | C | ARG | A | 320 | 37.750 | 37.319 | 35.223 | 1.00 | 21.22 | C |
| ATOM | 2463 | O | ARG | A | 320 | 37.669 | 37.210 | 36.439 | 1.00 | 21.65 | O |
| ATOM | 2464 | CB | ARG | A | 320 | 36.083 | 36.237 | 33.726 | 1.00 | 20.79 | C |
| ATOM | 2465 | CG | ARG | A | 320 | 34.702 | 36.243 | 33.014 | 1.00 | 22.36 | C |
| ATOM | 2466 | CD | ARG | A | 320 | 34.300 | 34.857 | 32.452 | 1.00 | 21.24 | C |
| ATOM | 2467 | NE | ARG | A | 320 | 34.147 | 33.910 | 33.558 | 1.00 | 21.37 | N |
| ATOM | 2468 | CZ | ARG | A | 320 | 33.148 | 33.957 | 34.423 | 1.00 | 21.73 | C |
| ATOM | 2469 | NH1 | ARG | A | 320 | 32.196 | 34.869 | 34.308 | 1.00 | 22.69 | N |
| ATOM | 2470 | NH2 | ARG | A | 320 | 33.100 | 33.109 | 35.425 | 1.00 | 23.33 | N |
| ATOM | 2471 | N | ASN | A | 321 | 38.908 | 37.216 | 34.571 | 1.00 | 21.35 | N |
| ATOM | 2472 | CA | ASN | A | 321 | 40.159 | 36.947 | 35.282 | 1.00 | 21.20 | C |
| ATOM | 2473 | C | ASN | A | 321 | 40.510 | 38.078 | 36.239 | 1.00 | 21.02 | C |
| ATOM | 2474 | O | ASN | A | 321 | 40.958 | 37.828 | 37.364 | 1.00 | 21.80 | O |
| ATOM | 2475 | CB | ASN | A | 321 | 41.314 | 36.648 | 34.311 | 1.00 | 21.07 | C |
| ATOM | 2476 | CG | ASN | A | 321 | 41.263 | 35.209 | 33.752 | 1.00 | 22.81 | C |
| ATOM | 2477 | OD1 | ASN | A | 321 | 40.821 | 34.306 | 34.431 | 1.00 | 23.88 | O |
| ATOM | 2478 | ND2 | ASN | A | 321 | 41.713 | 35.018 | 32.521 | 1.00 | 20.59 | N |
| ATOM | 2479 | N | ILE | A | 322 | 40.336 | 39.320 | 35.802 | 1.00 | 20.31 | N |
| ATOM | 2480 | CA | ILE | A | 322 | 40.611 | 40.447 | 36.683 | 1.00 | 19.83 | C |
| ATOM | 2481 | C | ILE | A | 322 | 39.721 | 40.344 | 37.918 | 1.00 | 19.45 | C |
| ATOM | 2482 | O | ILE | A | 322 | 40.178 | 40.531 | 39.037 | 1.00 | 18.04 | O |
| ATOM | 2483 | CB | ILE | A | 322 | 40.327 | 41.775 | 35.980 | 1.00 | 20.01 | C |
| ATOM | 2484 | CG1 | ILE | A | 322 | 41.320 | 42.009 | 34.849 | 1.00 | 21.62 | C |
| ATOM | 2485 | CG2 | ILE | A | 322 | 40.351 | 42.930 | 36.989 | 1.00 | 20.64 | C |
| ATOM | 2486 | CD1 | ILE | A | 322 | 42.782 | 41.987 | 35.278 | 1.00 | 23.99 | C |
| ATOM | 2487 | N | GLU | A | 323 | 38.444 | 40.035 | 37.716 | 1.00 | 18.87 | N |
| ATOM | 2488 | CA | GLU | A | 323 | 37.533 | 39.940 | 38.841 | 1.00 | 19.15 | C |
| ATOM | 2489 | C | GLU | A | 323 | 37.964 | 38.845 | 39.781 | 1.00 | 19.09 | C |
| ATOM | 2490 | O | GLU | A | 323 | 37.997 | 39.044 | 40.980 | 1.00 | 19.36 | O |
| ATOM | 2491 | CB | GLU | A | 323 | 36.095 | 39.721 | 38.366 | 1.00 | 19.19 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2492 | CG | GLU | A | 323 | 35.478 | 40.987 | 37.787 | 1.00 | 19.24 | C |
| ATOM | 2493 | CD | GLU | A | 323 | 34.096 | 40.764 | 37.189 | 1.00 | 17.51 | C |
| ATOM | 2494 | OE1 | GLU | A | 323 | 33.140 | 40.470 | 37.922 | 1.00 | 17.44 | O |
| ATOM | 2495 | OE2 | GLU | A | 323 | 33.982 | 40.901 | 35.974 | 1.00 | 16.60 | O |
| ATOM | 2496 | N | LYS | A | 324 | 38.357 | 37.711 | 39.227 | 1.00 | 19.47 | N |
| ATOM | 2497 | CA | LYS | A | 324 | 38.781 | 36.570 | 40.037 | 1.00 | 20.33 | C |
| ATOM | 2498 | C | LYS | A | 324 | 40.040 | 36.869 | 40.839 | 1.00 | 20.67 | C |
| ATOM | 2499 | O | LYS | A | 324 | 40.090 | 36.562 | 42.023 | 1.00 | 20.56 | O |
| ATOM | 2500 | CB | LYS | A | 324 | 39.040 | 35.334 | 39.172 | 1.00 | 20.11 | C |
| ATOM | 2501 | CG | LYS | A | 324 | 37.803 | 34.678 | 38.572 | 1.00 | 20.73 | C |
| ATOM | 2502 | CD | LYS | A | 324 | 38.238 | 33.413 | 37.761 | 1.00 | 21.68 | C |
| ATOM | 2503 | CE | LYS | A | 324 | 37.117 | 32.866 | 36.857 | 1.00 | 22.30 | C |
| ATOM | 2504 | NZ | LYS | A | 324 | 37.534 | 31.609 | 36.153 | 1.00 | 19.72 | N |
| ATOM | 2505 | N | MET | A | 325 | 41.045 | 37.456 | 40.194 | 1.00 | 21.37 | N |
| ATOM | 2506 | CA | MET | A | 325 | 42.305 | 37.782 | 40.860 | 1.00 | 22.78 | C |
| ATOM | 2507 | C | MET | A | 325 | 42.106 | 38.789 | 41.990 | 1.00 | 22.78 | C |
| ATOM | 2508 | O | MET | A | 325 | 42.734 | 38.694 | 43.047 | 1.00 | 22.48 | O |
| ATOM | 2509 | CB | MET | A | 325 | 43.308 | 38.369 | 39.865 | 1.00 | 23.14 | C |
| ATOM | 2510 | CG | MET | A | 325 | 43.964 | 37.359 | 38.978 | 1.00 | 27.30 | C |
| ATOM | 2511 | SD | MET | A | 325 | 44.699 | 38.147 | 37.511 | 1.00 | 35.72 | S |
| ATOM | 2512 | CE | MET | A | 325 | 45.804 | 39.221 | 38.338 | 1.00 | 36.16 | C |
| ATOM | 2513 | N | LEU | A | 326 | 41.248 | 39.765 | 41.752 | 1.00 | 23.21 | N |
| ATOM | 2514 | CA | LEU | A | 326 | 40.977 | 40.795 | 42.751 | 1.00 | 24.47 | C |
| ATOM | 2515 | C | LEU | A | 326 | 40.307 | 40.195 | 43.969 | 1.00 | 24.48 | C |
| ATOM | 2516 | O | LEU | A | 326 | 40.659 | 40.500 | 45.083 | 1.00 | 24.21 | O |
| ATOM | 2517 | CB | LEU | A | 326 | 40.087 | 41.863 | 42.159 | 1.00 | 24.63 | C |
| ATOM | 2518 | CG | LEU | A | 326 | 40.618 | 43.282 | 41.988 | 1.00 | 27.80 | C |
| ATOM | 2519 | CD1 | LEU | A | 326 | 42.135 | 43.441 | 42.036 | 1.00 | 28.29 | C |
| ATOM | 2520 | CD2 | LEU | A | 326 | 40.038 | 43.820 | 40.682 | 1.00 | 28.01 | C |
| ATOM | 2521 | N | GLY | A | 327 | 39.350 | 39.314 | 43.726 | 1.00 | 25.29 | N |
| ATOM | 2522 | CA | GLY | A | 327 | 38.663 | 38.608 | 44.782 | 1.00 | 25.73 | C |
| ATOM | 2523 | C | GLY | A | 327 | 39.644 | 37.854 | 45.638 | 1.00 | 25.86 | C |
| ATOM | 2524 | O | GLY | A | 327 | 39.597 | 37.931 | 46.863 | 1.00 | 25.83 | O |
| ATOM | 2525 | N | GLU | A | 328 | 40.556 | 37.137 | 45.002 | 1.00 | 26.02 | N |
| ATOM | 2526 | CA | GLU | A | 328 | 41.558 | 36.397 | 45.762 | 1.00 | 26.93 | C |
| ATOM | 2527 | C | GLU | A | 328 | 42.557 | 37.306 | 46.480 | 1.00 | 25.70 | C |
| ATOM | 2528 | O | GLU | A | 328 | 42.883 | 37.070 | 47.635 | 1.00 | 24.67 | O |
| ATOM | 2529 | CB | GLU | A | 328 | 42.293 | 35.423 | 44.853 | 1.00 | 27.76 | C |
| ATOM | 2530 | CG | GLU | A | 328 | 41.403 | 34.282 | 44.375 | 1.00 | 31.57 | C |
| ATOM | 2531 | CD | GLU | A | 328 | 41.635 | 32.992 | 45.146 | 1.00 | 37.39 | C |
| ATOM | 2532 | OE1 | GLU | A | 328 | 42.048 | 33.058 | 46.335 | 1.00 | 41.34 | O |
| ATOM | 2533 | OE2 | GLU | A | 328 | 41.430 | 31.902 | 44.552 | 1.00 | 42.69 | O |
| ATOM | 2534 | N | ALA | A | 329 | 43.024 | 38.356 | 45.816 | 1.00 | 25.20 | N |
| ATOM | 2535 | CA | ALA | A | 329 | 44.031 | 39.219 | 46.433 | 1.00 | 25.42 | C |
| ATOM | 2536 | C | ALA | A | 329 | 43.475 | 40.039 | 47.582 | 1.00 | 25.67 | C |
| ATOM | 2537 | O | ALA | A | 329 | 44.141 | 40.247 | 48.570 | 1.00 | 25.92 | O |
| ATOM | 2538 | CB | ALA | A | 329 | 44.670 | 40.109 | 45.409 | 1.00 | 25.31 | C |
| ATOM | 2539 | N | LEU | A | 330 | 42.241 | 40.496 | 47.467 | 1.00 | 26.51 | N |
| ATOM | 2540 | CA | LEU | A | 330 | 41.656 | 41.306 | 48.529 | 1.00 | 27.12 | C |
| ATOM | 2541 | C | LEU | A | 330 | 41.156 | 40.453 | 49.677 | 1.00 | 27.74 | C |
| ATOM | 2542 | O | LEU | A | 330 | 40.845 | 40.959 | 50.748 | 1.00 | 27.62 | O |
| ATOM | 2543 | CB | LEU | A | 330 | 40.517 | 42.138 | 47.984 | 1.00 | 27.19 | C |
| ATOM | 2544 | CG | LEU | A | 330 | 40.966 | 43.131 | 46.915 | 1.00 | 27.69 | C |
| ATOM | 2545 | CD1 | LEU | A | 330 | 39.747 | 43.661 | 46.211 | 1.00 | 28.15 | C |
| ATOM | 2546 | CD2 | LEU | A | 330 | 41.774 | 44.271 | 47.525 | 1.00 | 27.60 | C |
| ATOM | 2547 | N | GLY | A | 331 | 41.054 | 39.154 | 49.434 | 1.00 | 28.45 | N |
| ATOM | 2548 | CA | GLY | A | 331 | 40.637 | 38.222 | 50.457 | 1.00 | 29.04 | C |
| ATOM | 2549 | C | GLY | A | 331 | 39.154 | 38.239 | 50.748 | 1.00 | 29.16 | C |
| ATOM | 2550 | O | GLY | A | 331 | 38.698 | 37.505 | 51.615 | 1.00 | 29.67 | O |
| ATOM | 2551 | N | ASN | A | 332 | 38.409 | 39.088 | 50.052 | 1.00 | 29.16 | N |
| ATOM | 2552 | CA | ASN | A | 332 | 36.973 | 39.190 | 50.243 | 1.00 | 29.38 | C |

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ATOM   2553  C   ASN A 332      36.342  39.718  48.958  1.00 28.80           C
ATOM   2554  O   ASN A 332      36.579  40.847  48.570  1.00 28.58           O
ATOM   2555  CB  ASN A 332      36.662  40.123  51.413  1.00 29.68           C
ATOM   2556  CG  ASN A 332      35.181  40.214  51.702  1.00 31.38           C
ATOM   2557  OD1 ASN A 332      34.368  39.630  50.991  1.00 35.54           O
ATOM   2558  ND2 ASN A 332      34.820  40.944  52.751  1.00 33.23           N
ATOM   2559  N   PRO A 333      35.504  38.922  48.325  1.00 28.45           N
ATOM   2560  CA  PRO A 333      34.944  39.288  47.025  1.00 28.38           C
ATOM   2561  C   PRO A 333      34.094  40.534  47.093  1.00 28.04           C
ATOM   2562  O   PRO A 333      33.913  41.187  46.073  1.00 28.11           O
ATOM   2563  CB  PRO A 333      34.071  38.093  46.640  1.00 28.23           C
ATOM   2564  CG  PRO A 333      34.203  37.097  47.701  1.00 29.36           C
ATOM   2565  CD  PRO A 333      34.999  37.641  48.822  1.00 28.91           C
ATOM   2566  N   GLN A 334      33.556  40.844  48.262  1.00 27.75           N
ATOM   2567  CA  GLN A 334      32.727  42.033  48.400  1.00 28.08           C
ATOM   2568  C   GLN A 334      33.582  43.282  48.300  1.00 26.62           C
ATOM   2569  O   GLN A 334      33.064  44.365  48.086  1.00 26.31           O
ATOM   2570  CB  GLN A 334      31.857  41.989  49.686  1.00 28.89           C
ATOM   2571  CG  GLN A 334      30.594  41.090  49.459  1.00 32.52           C
ATOM   2572  CD  GLN A 334      29.523  41.114  50.556  1.00 36.22           C
ATOM   2573  OE1 GLN A 334      29.500  42.004  51.421  1.00 39.82           O
ATOM   2574  NE2 GLN A 334      28.612  40.127  50.503  1.00 38.24           N
ATOM   2575  N   GLU A 335      34.894  43.138  48.414  1.00 25.23           N
ATOM   2576  CA  GLU A 335      35.763  44.290  48.269  1.00 24.55           C
ATOM   2577  C   GLU A 335      36.090  44.584  46.790  1.00 22.95           C
ATOM   2578  O   GLU A 335      36.691  45.597  46.475  1.00 21.47           O
ATOM   2579  CB  GLU A 335      37.038  44.091  49.088  1.00 25.61           C
ATOM   2580  CG  GLU A 335      36.820  44.189  50.599  1.00 29.47           C
ATOM   2581  CD  GLU A 335      38.115  44.280  51.369  1.00 34.49           C
ATOM   2582  OE1 GLU A 335      38.964  45.124  51.004  1.00 39.50           O
ATOM   2583  OE2 GLU A 335      38.288  43.521  52.350  1.00 40.05           O
ATOM   2584  N   VAL A 336      35.654  43.722  45.877  1.00 21.52           N
ATOM   2585  CA  VAL A 336      35.993  43.898  44.458  1.00 20.69           C
ATOM   2586  C   VAL A 336      35.422  45.176  43.855  1.00 19.97           C
ATOM   2587  O   VAL A 336      36.134  45.949  43.239  1.00 19.57           O
ATOM   2588  CB  VAL A 336      35.594  42.683  43.653  1.00 20.59           C
ATOM   2589  CG1 VAL A 336      35.746  42.933  42.179  1.00 21.20           C
ATOM   2590  CG2 VAL A 336      36.467  41.513  44.067  1.00 21.28           C
ATOM   2591  N   GLY A 337      34.146  45.421  44.080  1.00 19.82           N
ATOM   2592  CA  GLY A 337      33.492  46.598  43.568  1.00 19.66           C
ATOM   2593  C   GLY A 337      34.130  47.906  43.981  1.00 19.56           C
ATOM   2594  O   GLY A 337      34.510  48.693  43.131  1.00 19.35           O
ATOM   2595  N   PRO A 338      34.202  48.162  45.278  1.00 19.93           N
ATOM   2596  CA  PRO A 338      34.846  49.383  45.790  1.00 19.88           C
ATOM   2597  C   PRO A 338      36.272  49.631  45.254  1.00 19.22           C
ATOM   2598  O   PRO A 338      36.591  50.758  44.908  1.00 18.43           O
ATOM   2599  CB  PRO A 338      34.830  49.191  47.316  1.00 19.61           C
ATOM   2600  CG  PRO A 338      33.625  48.380  47.555  1.00 20.33           C
ATOM   2601  CD  PRO A 338      33.579  47.367  46.359  1.00 20.75           C
ATOM   2602  N   LEU A 339      37.107  48.612  45.171  1.00 19.21           N
ATOM   2603  CA  LEU A 339      38.416  48.814  44.566  1.00 19.65           C
ATOM   2604  C   LEU A 339      38.283  49.219  43.081  1.00 19.35           C
ATOM   2605  O   LEU A 339      38.927  50.188  42.621  1.00 17.91           O
ATOM   2606  CB  LEU A 339      39.279  47.570  44.693  1.00 20.38           C
ATOM   2607  CG  LEU A 339      40.745  47.814  44.291  1.00 21.96           C
ATOM   2608  CD1 LEU A 339      41.681  47.151  45.220  1.00 25.12           C
ATOM   2609  CD2 LEU A 339      40.991  47.293  42.899  1.00 22.54           C
ATOM   2610  N   LEU A 340      37.420  48.512  42.345  1.00 19.18           N
ATOM   2611  CA  LEU A 340      37.231  48.821  40.928  1.00 19.26           C
ATOM   2612  C   LEU A 340      36.764  50.260  40.746  1.00 19.52           C
ATOM   2613  O   LEU A 340      37.306  50.989  39.893  1.00 18.71           O
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| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2614 | CB | LEU | A | 340 | 36.260 | 47.857 | 40.273 | 1.00 | 19.85 | C |
| ATOM | 2615 | CG | LEU | A | 340 | 36.823 | 46.470 | 39.960 | 1.00 | 21.77 | C |
| ATOM | 2616 | CD1 | LEU | A | 340 | 35.745 | 45.671 | 39.299 | 1.00 | 22.81 | C |
| ATOM | 2617 | CD2 | LEU | A | 340 | 38.088 | 46.539 | 39.072 | 1.00 | 21.14 | C |
| ATOM | 2618 | N | ASN | A | 341 | 35.798 | 50.676 | 41.570 | 1.00 | 19.12 | N |
| ATOM | 2619 | CA | ASN | A | 341 | 35.296 | 52.052 | 41.536 | 1.00 | 20.43 | C |
| ATOM | 2620 | C | ASN | A | 341 | 36.367 | 53.086 | 41.865 | 1.00 | 19.90 | C |
| ATOM | 2621 | O | ASN | A | 341 | 36.474 | 54.110 | 41.206 | 1.00 | 19.81 | O |
| ATOM | 2622 | CB | ASN | A | 341 | 34.090 | 52.232 | 42.485 | 1.00 | 20.40 | C |
| ATOM | 2623 | CG | ASN | A | 341 | 32.814 | 51.659 | 41.898 | 1.00 | 24.06 | C |
| ATOM | 2624 | OD1 | ASN | A | 341 | 32.390 | 52.073 | 40.829 | 1.00 | 31.36 | O |
| ATOM | 2625 | ND2 | ASN | A | 341 | 32.229 | 50.666 | 42.561 | 1.00 | 25.82 | N |
| ATOM | 2626 | N | THR | A | 342 | 37.129 | 52.812 | 42.912 | 1.00 | 19.43 | N |
| ATOM | 2627 | CA | THR | A | 342 | 38.227 | 53.664 | 43.305 | 1.00 | 19.71 | C |
| ATOM | 2628 | C | THR | A | 342 | 39.230 | 53.781 | 42.154 | 1.00 | 19.45 | C |
| ATOM | 2629 | O | THR | A | 342 | 39.739 | 54.859 | 41.893 | 1.00 | 19.23 | O |
| ATOM | 2630 | CB | THR | A | 342 | 38.873 | 53.073 | 44.555 | 1.00 | 20.44 | C |
| ATOM | 2631 | OG1 | THR | A | 342 | 38.030 | 53.322 | 45.700 | 1.00 | 21.13 | O |
| ATOM | 2632 | CG2 | THR | A | 342 | 40.208 | 53.756 | 44.874 | 1.00 | 20.71 | C |
| ATOM | 2633 | N | MET | A | 343 | 39.464 | 52.691 | 41.427 | 1.00 | 19.49 | N |
| ATOM | 2634 | CA | MET | A | 343 | 40.381 | 52.723 | 40.287 | 1.00 | 19.90 | C |
| ATOM | 2635 | C | MET | A | 343 | 39.932 | 53.649 | 39.164 | 1.00 | 19.94 | C |
| ATOM | 2636 | O | MET | A | 343 | 40.775 | 54.344 | 38.567 | 1.00 | 18.43 | O |
| ATOM | 2637 | CB | MET | A | 343 | 40.543 | 51.347 | 39.664 | 1.00 | 19.92 | C |
| ATOM | 2638 | CG | MET | A | 343 | 41.701 | 50.556 | 40.115 | 1.00 | 23.07 | C |
| ATOM | 2639 | SD | MET | A | 343 | 42.163 | 49.194 | 38.959 | 1.00 | 24.93 | S |
| ATOM | 2640 | CE | MET | A | 343 | 41.013 | 48.220 | 39.315 | 1.00 | 27.48 | C |
| ATOM | 2641 | N | ILE | A | 344 | 38.629 | 53.643 | 38.837 | 1.00 | 20.84 | N |
| ATOM | 2642 | CA | ILE | A | 344 | 38.159 | 54.412 | 37.679 | 1.00 | 21.51 | C |
| ATOM | 2643 | C | ILE | A | 344 | 37.624 | 55.800 | 37.918 | 1.00 | 21.46 | C |
| ATOM | 2644 | O | ILE | A | 344 | 37.751 | 56.639 | 37.018 | 1.00 | 21.65 | O |
| ATOM | 2645 | CB | ILE | A | 344 | 37.089 | 53.641 | 36.805 | 1.00 | 22.58 | C |
| ATOM | 2646 | CG1 | ILE | A | 344 | 35.714 | 53.723 | 37.435 | 1.00 | 24.65 | C |
| ATOM | 2647 | CG2 | ILE | A | 344 | 37.506 | 52.220 | 36.555 | 1.00 | 23.63 | C |
| ATOM | 2648 | CD1 | ILE | A | 344 | 34.635 | 53.407 | 36.511 | 1.00 | 28.35 | C |
| ATOM | 2649 | N | LYS | A | 345 | 37.009 | 56.092 | 39.062 | 1.00 | 21.48 | N |
| ATOM | 2650 | CA | LYS | A | 345 | 36.410 | 57.433 | 39.154 | 1.00 | 22.11 | C |
| ATOM | 2651 | C | LYS | A | 345 | 37.382 | 58.569 | 39.127 | 1.00 | 20.79 | C |
| ATOM | 2652 | O | LYS | A | 345 | 38.380 | 58.614 | 39.863 | 1.00 | 20.06 | O |
| ATOM | 2653 | CB | LYS | A | 345 | 35.405 | 57.656 | 40.279 | 1.00 | 23.49 | C |
| ATOM | 2654 | CG | LYS | A | 345 | 35.497 | 56.838 | 41.473 | 1.00 | 28.03 | C |
| ATOM | 2655 | CD | LYS | A | 345 | 34.120 | 56.183 | 41.683 | 1.00 | 30.07 | C |
| ATOM | 2656 | CE | LYS | A | 345 | 33.282 | 56.986 | 42.624 | 1.00 | 32.44 | C |
| ATOM | 2657 | NZ | LYS | A | 345 | 33.859 | 56.977 | 43.982 | 1.00 | 36.32 | N |
| ATOM | 2658 | N | GLY | A | 346 | 37.062 | 59.501 | 38.243 | 1.00 | 19.28 | N |
| ATOM | 2659 | CA | GLY | A | 346 | 37.911 | 60.636 | 38.013 | 1.00 | 18.60 | C |
| ATOM | 2660 | C | GLY | A | 346 | 39.222 | 60.254 | 37.350 | 1.00 | 17.41 | C |
| ATOM | 2661 | O | GLY | A | 346 | 40.090 | 61.079 | 37.229 | 1.00 | 18.04 | O |
| ATOM | 2662 | N | ARG | A | 347 | 39.353 | 59.024 | 36.898 | 1.00 | 17.62 | N |
| ATOM | 2663 | CA | ARG | A | 347 | 40.616 | 58.563 | 36.297 | 1.00 | 17.91 | C |
| ATOM | 2664 | C | ARG | A | 347 | 40.415 | 57.992 | 34.874 | 1.00 | 18.08 | C |
| ATOM | 2665 | O | ARG | A | 347 | 41.108 | 58.395 | 33.938 | 1.00 | 17.06 | O |
| ATOM | 2666 | CB | ARG | A | 347 | 41.284 | 57.532 | 37.213 | 1.00 | 17.51 | C |
| ATOM | 2667 | CG | ARG | A | 347 | 41.719 | 58.081 | 38.592 | 1.00 | 15.94 | C |
| ATOM | 2668 | CD | ARG | A | 347 | 43.179 | 57.649 | 38.985 | 1.00 | 19.49 | C |
| ATOM | 2669 | NE | ARG | A | 347 | 43.165 | 56.242 | 38.980 | 1.00 | 18.58 | N |
| ATOM | 2670 | CZ | ARG | A | 347 | 44.048 | 55.405 | 38.518 | 1.00 | 14.88 | C |
| ATOM | 2671 | NH1 | ARG | A | 347 | 45.271 | 55.726 | 38.085 | 1.00 | 17.47 | N |
| ATOM | 2672 | NH2 | ARG | A | 347 | 43.678 | 54.158 | 38.611 | 1.00 | 11.18 | N |
| ATOM | 2673 | N | TYR | A | 348 | 39.450 | 57.091 | 34.732 | 1.00 | 18.81 | N |
| ATOM | 2674 | CA | TYR | A | 348 | 39.098 | 56.480 | 33.444 | 1.00 | 20.50 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2675 | C | TYR | A | 348 | 37.637 | 56.691 | 33.036 | 1.00 22.07 | C |
| ATOM | 2676 | O | TYR | A | 348 | 37.233 | 56.236 | 31.978 | 1.00 22.11 | O |
| ATOM | 2677 | CB | TYR | A | 348 | 39.311 | 54.963 | 33.478 | 1.00 19.77 | C |
| ATOM | 2678 | CG | TYR | A | 348 | 40.753 | 54.545 | 33.561 | 1.00 20.36 | C |
| ATOM | 2679 | CD1 | TYR | A | 348 | 41.540 | 54.483 | 32.422 | 1.00 19.91 | C |
| ATOM | 2680 | CD2 | TYR | A | 348 | 41.335 | 54.225 | 34.780 | 1.00 18.20 | C |
| ATOM | 2681 | CE1 | TYR | A | 348 | 42.859 | 54.099 | 32.489 | 1.00 19.81 | C |
| ATOM | 2682 | CE2 | TYR | A | 348 | 42.662 | 53.841 | 34.863 | 1.00 19.47 | C |
| ATOM | 2683 | CZ | TYR | A | 348 | 43.425 | 53.785 | 33.711 | 1.00 19.43 | C |
| ATOM | 2684 | OH | TYR | A | 348 | 44.742 | 53.414 | 33.773 | 1.00 15.61 | O |
| ATOM | 2685 | N | ASN | A | 349 | 36.820 | 57.344 | 33.850 | 1.00 24.37 | N |
| ATOM | 2686 | CA | ASN | A | 349 | 35.414 | 57.472 | 33.456 | 1.00 26.66 | C |
| ATOM | 2687 | C | ASN | A | 349 | 34.941 | 58.854 | 33.092 | 1.00 28.03 | C |
| ATOM | 2688 | O | ASN | A | 349 | 35.663 | 59.847 | 32.992 | 1.00 27.79 | O |
| ATOM | 2689 | CB | ASN | A | 349 | 34.498 | 56.919 | 34.518 | 1.00 26.23 | C |
| ATOM | 2690 | CG | ASN | A | 349 | 34.463 | 57.764 | 35.748 | 1.00 27.89 | C |
| ATOM | 2691 | OD1 | ASN | A | 349 | 35.247 | 58.718 | 35.927 | 1.00 27.38 | O |
| ATOM | 2692 | ND2 | ASN | A | 349 | 33.545 | 57.409 | 36.645 | 1.00 32.46 | N |
| ATOM | 2693 | OXT | ASN | A | 349 | 33.736 | 58.963 | 32.900 | 1.00 32.44 | O |
| TER | 2694 | | ASN | A | 349 | | | | | |
| ATOM | 2695 | N | LEU | S | 795 | 45.819 | 35.786 | 30.984 | 1.00 36.91 | N |
| ATOM | 2696 | CA | LEU | S | 795 | 44.711 | 36.756 | 31.250 | 1.00 37.26 | C |
| ATOM | 2697 | C | LEU | S | 795 | 43.553 | 36.418 | 30.323 | 1.00 37.49 | C |
| ATOM | 2698 | O | LEU | S | 795 | 42.391 | 36.451 | 30.712 | 1.00 36.90 | O |
| ATOM | 2699 | CB | LEU | S | 795 | 45.183 | 38.186 | 31.044 | 1.00 37.26 | C |
| ATOM | 2700 | CG | LEU | S | 795 | 44.683 | 39.204 | 32.074 | 1.00 37.32 | C |
| ATOM | 2701 | CD1 | LEU | S | 795 | 44.775 | 38.671 | 33.479 | 1.00 37.34 | C |
| ATOM | 2702 | CD2 | LEU | S | 795 | 45.479 | 40.493 | 32.006 | 1.00 37.95 | C |
| ATOM | 2703 | N | THR | S | 796 | 43.907 | 36.155 | 29.076 | 1.00 38.07 | N |
| ATOM | 2704 | CA | THR | S | 796 | 43.029 | 35.548 | 28.076 | 1.00 39.17 | C |
| ATOM | 2705 | C | THR | S | 796 | 42.608 | 34.088 | 28.347 | 1.00 38.93 | C |
| ATOM | 2706 | O | THR | S | 796 | 41.784 | 33.533 | 27.622 | 1.00 39.51 | O |
| ATOM | 2707 | CB | THR | S | 796 | 43.750 | 35.628 | 26.705 | 1.00 39.45 | C |
| ATOM | 2708 | OG1 | THR | S | 796 | 43.287 | 34.597 | 25.850 | 1.00 41.87 | O |
| ATOM | 2709 | CG2 | THR | S | 796 | 45.232 | 35.275 | 26.824 | 1.00 40.14 | C |
| ATOM | 2710 | N | SER | S | 797 | 43.154 | 33.451 | 29.369 | 1.00 38.98 | N |
| ATOM | 2711 | CA | SER | S | 797 | 42.770 | 32.067 | 29.654 | 1.00 39.24 | C |
| ATOM | 2712 | C | SER | S | 797 | 41.370 | 31.981 | 30.274 | 1.00 39.32 | C |
| ATOM | 2713 | O | SER | S | 797 | 40.901 | 32.905 | 30.939 | 1.00 38.28 | O |
| ATOM | 2714 | CB | SER | S | 797 | 43.775 | 31.398 | 30.574 | 1.00 38.98 | C |
| ATOM | 2715 | OG | SER | S | 797 | 43.613 | 31.884 | 31.891 | 1.00 40.40 | O |
| ATOM | 2716 | N | TYR | S | 798 | 40.713 | 30.851 | 30.059 | 1.00 39.93 | N |
| ATOM | 2717 | CA | TYR | S | 798 | 39.345 | 30.682 | 30.515 | 1.00 40.53 | C |
| ATOM | 2718 | C | TYR | S | 798 | 39.088 | 29.350 | 31.183 | 1.00 39.72 | C |
| ATOM | 2719 | O | TYR | S | 798 | 39.797 | 28.383 | 30.958 | 1.00 39.72 | O |
| ATOM | 2720 | CB | TYR | S | 798 | 38.377 | 30.881 | 29.351 | 1.00 41.28 | C |
| ATOM | 2721 | CG | TYR | S | 798 | 38.524 | 29.939 | 28.171 | 1.00 44.57 | C |
| ATOM | 2722 | CD1 | TYR | S | 798 | 39.574 | 30.071 | 27.261 | 1.00 47.13 | C |
| ATOM | 2723 | CD2 | TYR | S | 798 | 37.574 | 28.953 | 27.932 | 1.00 47.85 | C |
| ATOM | 2724 | CE1 | TYR | S | 798 | 39.692 | 29.219 | 26.163 | 1.00 48.81 | C |
| ATOM | 2725 | CE2 | TYR | S | 798 | 37.680 | 28.094 | 26.833 | 1.00 50.32 | C |
| ATOM | 2726 | CZ | TYR | S | 798 | 38.744 | 28.229 | 25.955 | 1.00 49.97 | C |
| ATOM | 2727 | OH | TYR | S | 798 | 38.835 | 27.387 | 24.866 | 1.00 49.58 | O |
| ATOM | 2728 | N | ASP | S | 799 | 38.051 | 29.306 | 32.005 | 1.00 39.16 | N |
| ATOM | 2729 | CA | ASP | S | 799 | 37.676 | 28.076 | 32.690 | 1.00 38.61 | C |
| ATOM | 2730 | C | ASP | S | 799 | 36.588 | 27.391 | 31.868 | 1.00 37.26 | C |
| ATOM | 2731 | O | ASP | S | 799 | 36.468 | 27.657 | 30.671 | 1.00 36.81 | O |
| ATOM | 2732 | CB | ASP | S | 799 | 37.186 | 28.399 | 34.105 | 1.00 39.29 | C |
| ATOM | 2733 | CG | ASP | S | 799 | 37.303 | 27.223 | 35.048 | 1.00 40.55 | C |
| ATOM | 2734 | OD1 | ASP | S | 799 | 36.767 | 26.128 | 34.756 | 1.00 41.68 | O |
| ATOM | 2735 | OD2 | ASP | S | 799 | 37.913 | 27.319 | 36.121 | 1.00 45.38 | O |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2736 | N | CYS | S | 800 | 35.795 | 26.517 | 32.486 | 1.00 | 35.61 | N |
| ATOM | 2737 | CA | CYS | S | 800 | 34.781 | 25.787 | 31.732 | 1.00 | 34.66 | C |
| ATOM | 2738 | C | CYS | S | 800 | 33.439 | 25.714 | 32.450 | 1.00 | 34.03 | C |
| ATOM | 2739 | O | CYS | S | 800 | 32.749 | 24.708 | 32.388 | 1.00 | 33.81 | O |
| ATOM | 2740 | CB | CYS | S | 800 | 35.274 | 24.380 | 31.423 | 1.00 | 34.32 | C |
| ATOM | 2741 | SG | CYS | S | 800 | 35.538 | 23.392 | 32.911 | 1.00 | 33.88 | S |
| ATOM | 2742 | N | GLU | S | 801 | 33.051 | 26.792 | 33.101 | 1.00 | 33.69 | N |
| ATOM | 2743 | CA | GLU | S | 801 | 31.808 | 26.803 | 33.859 | 1.00 | 33.94 | C |
| ATOM | 2744 | C | GLU | S | 801 | 30.551 | 26.980 | 32.991 | 1.00 | 33.69 | C |
| ATOM | 2745 | O | GLU | S | 801 | 30.520 | 27.739 | 32.012 | 1.00 | 32.67 | O |
| ATOM | 2746 | CB | GLU | S | 801 | 31.886 | 27.877 | 34.942 | 1.00 | 34.03 | C |
| ATOM | 2747 | CG | GLU | S | 801 | 33.128 | 27.703 | 35.818 | 1.00 | 36.03 | C |
| ATOM | 2748 | CD | GLU | S | 801 | 33.095 | 28.557 | 37.065 | 1.00 | 36.15 | C |
| ATOM | 2749 | OE1 | GLU | S | 801 | 32.408 | 28.163 | 38.013 | 1.00 | 35.62 | O |
| ATOM | 2750 | OE2 | GLU | S | 801 | 33.751 | 29.619 | 37.090 | 1.00 | 38.69 | O |
| ATOM | 2751 | N | VAL | S | 802 | 29.519 | 26.242 | 33.377 | 1.00 | 33.95 | N |
| ATOM | 2752 | CA | VAL | S | 802 | 28.244 | 26.223 | 32.691 | 1.00 | 33.82 | C |
| ATOM | 2753 | C | VAL | S | 802 | 27.137 | 26.148 | 33.735 | 1.00 | 34.17 | C |
| ATOM | 2754 | O | VAL | S | 802 | 27.408 | 25.928 | 34.908 | 1.00 | 33.56 | O |
| ATOM | 2755 | CB | VAL | S | 802 | 28.139 | 24.972 | 31.781 | 1.00 | 33.63 | C |
| ATOM | 2756 | CG1 | VAL | S | 802 | 29.263 | 24.948 | 30.753 | 1.00 | 32.61 | C |
| ATOM | 2757 | CG2 | VAL | S | 802 | 28.165 | 23.682 | 32.624 | 1.00 | 33.77 | C |
| ATOM | 2758 | N | ASN | S | 803 | 25.887 | 26.304 | 33.300 | 1.00 | 35.05 | N |
| ATOM | 2759 | CA | ASN | S | 803 | 24.745 | 26.222 | 34.204 | 1.00 | 35.82 | C |
| ATOM | 2760 | C | ASN | S | 803 | 24.457 | 24.784 | 34.642 | 1.00 | 37.45 | C |
| ATOM | 2761 | O | ASN | S | 803 | 23.379 | 24.241 | 34.387 | 1.00 | 37.12 | O |
| ATOM | 2762 | CB | ASN | S | 803 | 23.490 | 26.836 | 33.573 | 1.00 | 35.36 | C |
| ATOM | 2763 | CG | ASN | S | 803 | 23.548 | 28.344 | 33.506 | 1.00 | 33.54 | C |
| ATOM | 2764 | OD1 | ASN | S | 803 | 24.605 | 28.941 | 33.685 | 1.00 | 32.05 | O |
| ATOM | 2765 | ND2 | ASN | S | 803 | 22.414 | 28.967 | 33.230 | 1.00 | 29.41 | N |
| ATOM | 2766 | N | ALA | S | 804 | 25.442 | 24.187 | 35.298 | 1.00 | 39.28 | N |
| ATOM | 2767 | CA | ALA | S | 804 | 25.340 | 22.846 | 35.855 | 1.00 | 41.13 | C |
| ATOM | 2768 | C | ALA | S | 804 | 26.566 | 22.620 | 36.734 | 1.00 | 42.43 | C |
| ATOM | 2769 | O | ALA | S | 804 | 27.638 | 23.153 | 36.464 | 1.00 | 42.47 | O |
| ATOM | 2770 | CB | ALA | S | 804 | 25.277 | 21.791 | 34.762 | 1.00 | 41.08 | C |
| ATOM | 2771 | N | PRO | S | 805 | 26.410 | 21.830 | 37.786 | 1.00 | 44.47 | N |
| ATOM | 2772 | CA | PRO | S | 805 | 27.527 | 21.527 | 38.697 | 1.00 | 45.68 | C |
| ATOM | 2773 | C | PRO | S | 805 | 28.568 | 20.620 | 38.053 | 1.00 | 46.82 | C |
| ATOM | 2774 | O | PRO | S | 805 | 28.273 | 19.918 | 37.092 | 1.00 | 47.40 | O |
| ATOM | 2775 | CB | PRO | S | 805 | 26.847 | 20.783 | 39.854 | 1.00 | 45.66 | C |
| ATOM | 2776 | CG | PRO | S | 805 | 25.588 | 20.206 | 39.261 | 1.00 | 45.01 | C |
| ATOM | 2777 | CD | PRO | S | 805 | 25.161 | 21.146 | 38.177 | 1.00 | 44.63 | C |
| ATOM | 2778 | N | ILE | S | 806 | 29.770 | 20.613 | 38.605 | 1.00 | 48.31 | N |
| ATOM | 2779 | CA | ILE | S | 806 | 30.847 | 19.766 | 38.098 | 1.00 | 49.34 | C |
| ATOM | 2780 | C | ILE | S | 806 | 30.661 | 18.323 | 38.555 | 1.00 | 49.57 | C |
| ATOM | 2781 | O | ILE | S | 806 | 29.992 | 18.063 | 39.560 | 1.00 | 50.13 | O |
| ATOM | 2782 | CB | ILE | S | 806 | 32.215 | 20.311 | 38.574 | 1.00 | 49.85 | C |
| ATOM | 2783 | CG1 | ILE | S | 806 | 32.410 | 20.058 | 40.074 | 1.00 | 50.64 | C |
| ATOM | 2784 | CG2 | ILE | S | 806 | 32.327 | 21.816 | 38.250 | 1.00 | 50.45 | C |
| ATOM | 2785 | CD1 | ILE | S | 806 | 33.724 | 20.605 | 40.624 | 1.00 | 51.43 | C |
| ATOM | 2786 | N | LEU | S | 813 | 29.871 | 8.315 | 36.218 | 1.00 | 46.23 | N |
| ATOM | 2787 | CA | LEU | S | 813 | 30.588 | 8.788 | 35.034 | 1.00 | 46.32 | C |
| ATOM | 2788 | C | LEU | S | 813 | 29.685 | 9.635 | 34.140 | 1.00 | 45.87 | C |
| ATOM | 2789 | O | LEU | S | 813 | 28.463 | 9.511 | 34.185 | 1.00 | 45.43 | O |
| ATOM | 2790 | CB | LEU | S | 813 | 31.166 | 7.606 | 34.243 | 1.00 | 46.25 | C |
| ATOM | 2791 | CG | LEU | S | 813 | 32.057 | 6.663 | 35.059 | 1.00 | 46.61 | C |
| ATOM | 2792 | CD1 | LEU | S | 813 | 32.444 | 5.423 | 34.230 | 1.00 | 46.51 | C |
| ATOM | 2793 | CD2 | LEU | S | 813 | 33.292 | 7.406 | 35.579 | 1.00 | 45.98 | C |
| ATOM | 2794 | N | GLN | S | 814 | 30.309 | 10.503 | 33.351 | 1.00 | 45.81 | N |
| ATOM | 2795 | CA | GLN | S | 814 | 29.595 | 11.400 | 32.446 | 1.00 | 45.92 | C |
| ATOM | 2796 | C | GLN | S | 814 | 30.497 | 11.838 | 31.296 | 1.00 | 45.66 | C |

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ATOM   2797  O   GLN S 814      31.706  11.626  31.329  1.00 45.05           O
ATOM   2798  CB  GLN S 814      29.123  12.643  33.198  1.00 46.09           C
ATOM   2799  CG  GLN S 814      30.265  13.531  33.696  1.00 47.32           C
ATOM   2800  CD  GLN S 814      29.781  14.722  34.520  1.00 49.22           C
ATOM   2801  OE1 GLN S 814      29.165  14.541  35.569  1.00 50.40           O
ATOM   2802  NE2 GLN S 814      30.070  15.937  34.053  1.00 49.45           N
ATOM   2803  N   GLY S 815      29.898  12.476  30.294  1.00 45.88           N
ATOM   2804  CA  GLY S 815      30.621  12.956  29.135  1.00 45.84           C
ATOM   2805  C   GLY S 815      31.426  11.863  28.462  1.00 46.13           C
ATOM   2806  O   GLY S 815      30.968  10.732  28.339  1.00 45.49           O
ATOM   2807  N   GLU S 816      32.633  12.216  28.035  1.00 46.94           N
ATOM   2808  CA  GLU S 816      33.548  11.285  27.382  1.00 48.03           C
ATOM   2809  C   GLU S 816      33.721   9.994  28.186  1.00 48.62           C
ATOM   2810  O   GLU S 816      33.823   8.910  27.614  1.00 48.54           O
ATOM   2811  CB  GLU S 816      34.920  11.948  27.184  1.00 48.06           C
ATOM   2812  CG  GLU S 816      35.783  11.312  26.102  1.00 48.93           C
ATOM   2813  CD  GLU S 816      37.189  11.887  26.062  1.00 49.77           C
ATOM   2814  OE1 GLU S 816      38.031  11.413  26.848  1.00 50.86           O
ATOM   2815  OE2 GLU S 816      37.457  12.802  25.247  1.00 49.55           O
ATOM   2816  N   GLU S 817      33.737  10.112  29.509  1.00 49.67           N
ATOM   2817  CA  GLU S 817      33.947   8.957  30.373  1.00 50.75           C
ATOM   2818  C   GLU S 817      32.786   7.982  30.309  1.00 51.10           C
ATOM   2819  O   GLU S 817      32.989   6.771  30.278  1.00 51.12           O
ATOM   2820  CB  GLU S 817      34.164   9.406  31.815  1.00 50.97           C
ATOM   2821  CG  GLU S 817      35.476  10.140  32.032  1.00 52.22           C
ATOM   2822  CD  GLU S 817      35.395  11.637  31.764  1.00 54.47           C
ATOM   2823  OE1 GLU S 817      34.289  12.166  31.489  1.00 55.57           O
ATOM   2824  OE2 GLU S 817      36.456  12.296  31.833  1.00 56.41           O
ATOM   2825  N   LEU S 818      31.572   8.521  30.295  1.00 51.81           N
ATOM   2826  CA  LEU S 818      30.376   7.706  30.204  1.00 52.37           C
ATOM   2827  C   LEU S 818      30.399   6.929  28.901  1.00 53.14           C
ATOM   2828  O   LEU S 818      30.216   5.714  28.894  1.00 53.00           O
ATOM   2829  CB  LEU S 818      29.116   8.575  30.258  1.00 52.25           C
ATOM   2830  CG  LEU S 818      27.786   7.814  30.176  1.00 52.17           C
ATOM   2831  CD1 LEU S 818      27.661   6.836  31.335  1.00 52.37           C
ATOM   2832  CD2 LEU S 818      26.596   8.749  30.173  1.00 51.16           C
ATOM   2833  N   LEU S 819      30.660   7.643  27.809  1.00 54.00           N
ATOM   2834  CA  LEU S 819      30.623   7.068  26.465  1.00 54.73           C
ATOM   2835  C   LEU S 819      31.573   5.874  26.295  1.00 55.32           C
ATOM   2836  O   LEU S 819      31.171   4.823  25.794  1.00 55.08           O
ATOM   2837  CB  LEU S 819      30.929   8.162  25.426  1.00 54.66           C
ATOM   2838  CG  LEU S 819      30.838   7.789  23.942  1.00 54.90           C
ATOM   2839  CD1 LEU S 819      29.480   7.239  23.559  1.00 54.56           C
ATOM   2840  CD2 LEU S 819      31.170   8.997  23.088  1.00 55.68           C
ATOM   2841  N   ARG S 820      32.821   6.036  26.725  1.00 55.92           N
ATOM   2842  CA  ARG S 820      33.817   4.987  26.576  1.00 56.75           C
ATOM   2843  C   ARG S 820      33.488   3.762  27.428  1.00 56.92           C
ATOM   2844  O   ARG S 820      33.578   2.617  26.951  1.00 56.86           O
ATOM   2845  CB  ARG S 820      35.207   5.530  26.915  1.00 57.13           C
ATOM   2846  CG  ARG S 820      35.638   6.596  25.927  1.00 58.55           C
ATOM   2847  CD  ARG S 820      37.073   7.038  26.036  1.00 60.19           C
ATOM   2848  NE  ARG S 820      37.336   8.126  25.096  1.00 62.23           N
ATOM   2849  CZ  ARG S 820      38.465   8.831  25.039  1.00 64.08           C
ATOM   2850  NH1 ARG S 820      39.475   8.567  25.865  1.00 64.81           N
ATOM   2851  NH2 ARG S 820      38.586   9.805  24.142  1.00 64.58           N
ATOM   2852  N   ALA S 821      33.109   4.003  28.682  1.00 56.90           N
ATOM   2853  CA  ALA S 821      32.713   2.919  29.567  1.00 56.79           C
ATOM   2854  C   ALA S 821      31.611   2.106  28.880  1.00 56.74           C
ATOM   2855  O   ALA S 821      31.665   0.873  28.843  1.00 56.66           O
ATOM   2856  CB  ALA S 821      32.236   3.463  30.899  1.00 56.66           C
ATOM   2857  N   LEU S 822      30.629   2.806  28.317  1.00 56.51           N
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ATOM   2858  CA  LEU S 822      29.537   2.155  27.607  1.00 56.58           C
ATOM   2859  C   LEU S 822      30.031   1.473  26.338  1.00 56.66           C
ATOM   2860  O   LEU S 822      29.482   0.451  25.931  1.00 57.09           O
ATOM   2861  CB  LEU S 822      28.451   3.167  27.250  1.00 56.48           C
ATOM   2862  CG  LEU S 822      27.681   3.779  28.417  1.00 56.11           C
ATOM   2863  CD1 LEU S 822      26.543   4.612  27.870  1.00 55.96           C
ATOM   2864  CD2 LEU S 822      27.156   2.717  29.379  1.00 55.80           C
TER    2865      LEU S 822
HETATM 2866 FE   FE2 A1350      23.313  27.671  28.779  1.00 22.12          FE
HETATM 2867  C1  AKG A1351      22.355  25.315  27.747  1.00 25.61           C
HETATM 2868  O1  AKG A1351      23.449  25.880  27.756  1.00 27.58           O
HETATM 2869  O2  AKG A1351      22.172  24.103  27.197  1.00 27.99           O
HETATM 2870  C2  AKG A1351      21.128  25.999  28.365  1.00 24.14           C
HETATM 2871  O5  AKG A1351      21.211  27.117  28.854  1.00 23.66           O
HETATM 2872  C3  AKG A1351      19.829  25.231  28.280  1.00 23.46           C
HETATM 2873  C4  AKG A1351      18.717  25.967  29.008  1.00 22.15           C
HETATM 2874  C5  AKG A1351      17.351  25.435  28.649  1.00 23.90           C
HETATM 2875  O3  AKG A1351      17.136  24.674  27.706  1.00 23.27           O
HETATM 2876  O4  AKG A1351      16.353  25.844  29.406  1.00 25.34           O
HETATM 2877  S   SO4 A1352       0.196  25.255  43.681  1.00 83.69           S
HETATM 2878  O1  SO4 A1352       1.049  26.078  44.531  1.00 83.03           O
HETATM 2879  O2  SO4 A1352       1.028  24.391  42.840  1.00 82.84           O
HETATM 2880  O3  SO4 A1352      -0.643  24.431  44.542  1.00 83.90           O
HETATM 2881  O4  SO4 A1352      -0.630  26.114  42.830  1.00 82.82           O
HETATM 2882  S   SO4 A1353       1.937  28.607  29.759  1.00 80.69           S
HETATM 2883  O1  SO4 A1353       3.164  29.179  30.298  1.00 79.82           O
HETATM 2884  O2  SO4 A1353       2.228  27.552  28.793  1.00 79.89           O
HETATM 2885  O3  SO4 A1353       1.188  28.079  30.902  1.00 82.14           O
HETATM 2886  O4  SO4 A1353       1.145  29.630  29.081  1.00 81.49           O
HETATM 2887  O   HOH H   1      38.423  33.864  31.899  1.00 39.52           O
HETATM 2888  O   HOH H   2      38.025  25.366  29.554  1.00 64.59           O
HETATM 2889  O   HOH H   3      34.915  30.689  35.190  1.00 34.36           O
HETATM 2890  O   HOH H   4      20.482  27.037  33.306  1.00 55.20           O
HETATM 2891  O   HOH H   5      21.066  24.447  32.916  1.00 43.55           O
HETATM 2892  O   HOH H   6      29.978  24.394  35.721  1.00 43.81           O
HETATM 2893  O   HOH H   7      29.346  18.985  42.744  1.00 86.25           O
HETATM 2894  O   HOH H   8      35.530  13.904  24.157  1.00 42.65           O
HETATM 2895  O   HOH H   9      33.804  -1.383  26.877  1.00 65.05           O
HETATM 2896  O   HOH Z   1      11.560  21.626  13.846  1.00 41.47           O
HETATM 2897  O   HOH Z   2       9.590  21.877  12.314  1.00 61.59           O
HETATM 2898  O   HOH Z   3       1.321  21.339   7.657  1.00 58.53           O
HETATM 2899  O   HOH Z   4       3.579  13.365   8.778  1.00 47.77           O
HETATM 2900  O   HOH Z   5       4.515  16.855   3.766  1.00 51.50           O
HETATM 2901  O   HOH Z   6       2.462  19.552   5.161  1.00 56.40           O
HETATM 2902  O   HOH Z   7       1.251  29.413  13.184  1.00 52.18           O
HETATM 2903  O   HOH Z   8       2.053  32.304  13.875  1.00 71.43           O
HETATM 2904  O   HOH Z   9      11.574  44.907  14.867  1.00 67.18           O
HETATM 2905  O   HOH Z  10      11.615   3.238  17.221  1.00 63.99           O
HETATM 2906  O   HOH Z  11       3.752  32.951  32.375  1.00 72.66           O
HETATM 2907  O   HOH Z  12       4.803  37.611  27.421  1.00 63.47           O
HETATM 2908  O   HOH Z  13      11.007  35.734  30.393  1.00 34.95           O
HETATM 2909  O   HOH Z  14      15.551  46.392  24.481  1.00 43.01           O
HETATM 2910  O   HOH Z  15      12.231  41.979  15.720  1.00 53.94           O
HETATM 2911  O   HOH Z  16      13.868   4.815  17.661  1.00 48.46           O
HETATM 2912  O   HOH Z  17      15.860  30.606  12.755  1.00 44.45           O
HETATM 2913  O   HOH Z  18      13.462  22.030   7.390  1.00 59.18           O
HETATM 2914  O   HOH Z  19      14.706  26.336  13.845  1.00 51.42           O
HETATM 2915  O   HOH Z  20      17.028  29.994   7.603  1.00 64.07           O
HETATM 2916  O   HOH Z  21      21.135  23.988   3.773  1.00 46.32           O
HETATM 2917  O   HOH Z  22      27.581  31.130   6.026  1.00 64.13           O
HETATM 2918  O   HOH Z  23      27.341  22.242  43.414  1.00 79.43           O
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HETATM 2919  O   HOH Z  24      36.742  29.331  21.279  1.00 50.70           O
HETATM 2920  O   HOH Z  25      30.029  33.533   9.206  1.00 50.33           O
HETATM 2921  O   HOH Z  26      29.955  37.104  10.551  1.00 70.40           O
HETATM 2922  O   HOH Z  27      18.215  15.129  13.036  1.00 37.33           O
HETATM 2923  O   HOH Z  28      29.069   5.533  17.355  1.00 44.84           O
HETATM 2924  O   HOH Z  29      18.941  14.771  16.383  1.00 31.41           O
HETATM 2925  O   HOH Z  30      13.624   7.655  18.343  1.00 46.45           O
HETATM 2926  O   HOH Z  31       5.649  12.667  27.758  1.00 44.15           O
HETATM 2927  O   HOH Z  32      18.818   6.772  36.717  1.00 51.59           O
HETATM 2928  O   HOH Z  33       7.620  14.589  19.463  1.00 50.93           O
HETATM 2929  O   HOH Z  34      20.087   9.746  36.974  1.00 52.81           O
HETATM 2930  O   HOH Z  35      21.912  13.173  44.511  1.00 59.64           O
HETATM 2931  O   HOH Z  36      29.233  39.992  16.108  1.00 75.75           O
HETATM 2932  O   HOH Z  37      33.785  44.067  25.671  1.00 62.06           O
HETATM 2933  O   HOH Z  38      15.613  37.779  35.493  1.00 52.50           O
HETATM 2934  O   HOH Z  39       8.070  38.292  35.056  1.00 60.61           O
HETATM 2935  O   HOH Z  40      16.339  30.957  40.378  1.00 43.15           O
HETATM 2936  O   HOH Z  41      28.116  27.147  37.617  1.00 59.20           O
HETATM 2937  O   HOH Z  42      29.707  30.087  39.279  1.00 54.89           O
HETATM 2938  O   HOH Z  43      28.116  24.509  42.048  1.00 63.13           O
HETATM 2939  O   HOH Z  44      25.074  24.801  42.258  1.00 54.81           O
HETATM 2940  O   HOH Z  45      33.873  31.493  39.077  1.00 45.97           O
HETATM 2941  O   HOH Z  46      31.533  33.860  46.118  1.00 50.65           O
HETATM 2942  O   HOH Z  47      13.319  35.957  31.390  1.00 44.72           O
HETATM 2943  O   HOH Z  48      27.155  38.119  52.311  1.00 64.05           O
HETATM 2944  O   HOH Z  49      24.587  38.767  49.612  1.00 50.58           O
HETATM 2945  O   HOH Z  50      21.687  17.630  48.071  1.00 77.36           O
HETATM 2946  O   HOH Z  51      21.437  14.872  40.880  1.00 60.20           O
HETATM 2947  O   HOH Z  52      24.790  15.406  39.359  1.00 78.81           O
HETATM 2948  O   HOH Z  53      23.347  17.356  36.625  1.00 52.48           O
HETATM 2949  O   HOH Z  54      21.628  10.475  34.469  1.00 47.30           O
HETATM 2950  O   HOH Z  55      18.013  -1.527  33.036  1.00 61.93           O
HETATM 2951  O   HOH Z  56      16.101  -0.104  30.078  1.00 59.33           O
HETATM 2952  O   HOH Z  57      26.268   5.539  16.988  1.00 38.42           O
HETATM 2953  O   HOH Z  58      30.916  16.527  11.437  1.00 44.01           O
HETATM 2954  O   HOH Z  59      32.683  13.953  20.664  1.00 50.04           O
HETATM 2955  O   HOH Z  60      36.797  10.766   7.771  1.00 80.75           O
HETATM 2956  O   HOH Z  61      33.878  26.222  17.133  1.00 45.23           O
HETATM 2957  O   HOH Z  62      13.442  21.089  28.459  1.00 36.04           O
HETATM 2958  O   HOH Z  63       3.999  21.370  30.471  1.00 47.33           O
HETATM 2959  O   HOH Z  64      30.697  38.141  33.290  1.00 31.70           O
HETATM 2960  O   HOH Z  65      26.005  26.456  26.227  1.00 28.76           O
HETATM 2961  O   HOH Z  66      36.729  32.146  33.280  1.00 42.61           O
HETATM 2962  O   HOH Z  67      35.846  25.574  27.896  1.00 34.95           O
HETATM 2963  O   HOH Z  68      36.793  26.712  21.173  1.00 33.97           O
HETATM 2964  O   HOH Z  69      17.427  17.022  18.148  1.00 31.28           O
HETATM 2965  O   HOH Z  70       9.904  13.694  19.533  1.00 41.70           O
HETATM 2966  O   HOH Z  71       5.361  16.931  22.051  1.00 43.04           O
HETATM 2967  O   HOH Z  72       7.094  16.984  20.250  1.00 43.57           O
HETATM 2968  O   HOH Z  73       6.562  22.961  22.902  1.00 42.74           O
HETATM 2969  O   HOH Z  74      29.508  38.942  26.471  1.00 26.72           O
HETATM 2970  O   HOH Z  75      30.732  39.209  19.135  1.00 37.64           O
HETATM 2971  O   HOH Z  76      26.368  42.318  17.836  1.00 57.14           O
HETATM 2972  O   HOH Z  77      27.688  44.616  31.257  1.00 30.61           O
HETATM 2973  O   HOH Z  78      30.230  44.988  25.170  1.00 39.14           O
HETATM 2974  O   HOH Z  79      27.780  48.720  30.030  1.00 38.89           O
HETATM 2975  O   HOH Z  80      25.931  50.741  30.611  1.00 40.27           O
HETATM 2976  O   HOH Z  81      18.521  38.529  36.775  1.00 43.87           O
HETATM 2977  O   HOH Z  82      26.678  31.402  38.482  1.00 36.08           O
HETATM 2978  O   HOH Z  83      30.586  30.409  36.592  1.00 32.57           O
HETATM 2979  O   HOH Z  84      29.411  37.141  35.473  1.00 26.16           O
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HETATM 2980  O   HOH Z  85      19.821  31.713  33.874  1.00 34.80           O
HETATM 2981  O   HOH Z  86      19.420  36.322  33.379  1.00 32.92           O
HETATM 2982  O   HOH Z  87      21.063  42.853  40.110  1.00 41.23           O
HETATM 2983  O   HOH Z  88      17.544  37.859  32.276  1.00 35.87           O
HETATM 2984  O   HOH Z  89       9.230  41.082  35.833  1.00 51.41           O
HETATM 2985  O   HOH Z  90       9.313  43.744  27.890  1.00 70.60           O
HETATM 2986  O   HOH Z  91      12.728  42.598  26.938  1.00 40.87           O
HETATM 2987  O   HOH Z  92      15.113  37.993  32.591  1.00 35.55           O
HETATM 2988  O   HOH Z  93      10.676  48.283  31.613  1.00 62.24           O
HETATM 2989  O   HOH Z  94      15.611  44.853  34.883  1.00 32.72           O
HETATM 2990  O   HOH Z  95      15.874  51.836  39.217  1.00 66.58           O
HETATM 2991  O   HOH Z  96      15.796  47.224  39.264  1.00 52.95           O
HETATM 2992  O   HOH Z  97      26.624  53.557  28.816  1.00 69.05           O
HETATM 2993  O   HOH Z  98      15.381  50.418  22.170  1.00 36.68           O
HETATM 2994  O   HOH Z  99      15.121  55.730  27.489  1.00 51.35           O
HETATM 2995  O   HOH Z 100      18.542  56.170  28.175  1.00 58.02           O
HETATM 2996  O   HOH Z 101      23.731  46.355  19.907  1.00 39.06           O
HETATM 2997  O   HOH Z 102      16.618  46.781  22.039  1.00 33.91           O
HETATM 2998  O   HOH Z 103      26.585  40.624  15.634  1.00 69.17           O
HETATM 2999  O   HOH Z 104      12.758  29.333  13.489  1.00 35.42           O
HETATM 3000  O   HOH Z 105      10.886  19.245  14.132  1.00 51.89           O
HETATM 3001  O   HOH Z 106      19.776  18.049  13.245  1.00 33.88           O
HETATM 3002  O   HOH Z 107      14.725  18.642  12.190  1.00 40.50           O
HETATM 3003  O   HOH Z 108      27.783  27.681  24.556  1.00 27.24           O
HETATM 3004  O   HOH Z 109      35.999  32.896  30.270  1.00 41.19           O
HETATM 3005  O   HOH Z 110      30.237  36.282  26.881  1.00 28.77           O
HETATM 3006  O   HOH Z 111      32.759  34.258  19.346  1.00 47.40           O
HETATM 3007  O   HOH Z 112      27.418  30.315  25.756  1.00 27.70           O
HETATM 3008  O   HOH Z 113      16.248  36.360  29.657  1.00 34.03           O
HETATM 3009  O   HOH Z 114       7.438  31.072  24.792  1.00 43.13           O
HETATM 3010  O   HOH Z 115       7.743  30.565  27.379  1.00 39.83           O
HETATM 3011  O   HOH Z 116       5.158  19.080  24.012  1.00 45.77           O
HETATM 3012  O   HOH Z 117       6.366  24.013  25.459  1.00 41.84           O
HETATM 3013  O   HOH Z 118      42.594  37.813  18.527  1.00 64.57           O
HETATM 3014  O   HOH Z 119      42.361  44.340  19.742  1.00 59.24           O
HETATM 3015  O   HOH Z 120      34.674  39.749  17.782  1.00 53.99           O
HETATM 3016  O   HOH Z 121      33.762  37.015  20.310  1.00 39.85           O
HETATM 3017  O   HOH Z 122      33.121  39.446  33.667  1.00 30.35           O
HETATM 3018  O   HOH Z 123      37.674  29.865  38.229  1.00 64.32           O
HETATM 3019  O   HOH Z 124      38.677  34.824  42.977  1.00 44.37           O
HETATM 3020  O   HOH Z 125      41.375  43.570  51.489  1.00 52.41           O
HETATM 3021  O   HOH Z 126      31.947  40.559  44.192  1.00 38.39           O
HETATM 3022  O   HOH Z 127      39.124  57.396  42.134  1.00 27.12           O
HETATM 3023  O   HOH Z 128      41.949  60.812  33.590  1.00 49.78           O
HETATM 3024  O   HOH Z 129      46.835  53.394  32.063  1.00 33.50           O
HETATM 3025  O   HOH Z 130      37.841  55.408  29.621  1.00 45.14           O
CONECT 1482 2866
CONECT 1502 2866
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CONECT 2878 2877
CONECT 2879 2877
CONECT 2880 2877
CONECT 2881 2877
CONECT 2882 2883 2884 2885 2886
CONECT 2883 2882
CONECT 2884 2882
CONECT 2885 2882
CONECT 2886 2882
MASTER      437    0    4   15   20    0    7    6 3023    2   24   31
END
```

Structure 3

Below are the coordinates for structure 3 (the 2.5 Å structure of FIH:Zn(II):NOG:CAD):

```
HEADER    TRANSCRIPTION ACTIVATOR/INHIBITOR       12-AUG-02   1H2M
TITLE     FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE    2 FRAGMENT PEPTIDE
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND   3 SYNONYM: FIH1;
COMPND   4 CHAIN: A;
COMPND   5 ENGINEERED: YES;
COMPND   6 MOL_ID: 2;
COMPND   7 MOLECULE: HYPOXIA-INDUCIBLE FACTOR 1 ALPHA;
COMPND   8 SYNONYM: HIF-1 ALPHA, ARNT INTERACTING PROTEIN,
COMPND   9  MEMBER OF PAS PROTEIN 1, MOP1, HIF1 ALPHA, HIF1A.
COMPND  10 CHAIN: S;
COMPND  11 FRAGMENT: C-TERMINAL TRANSACTIVATION DOMAIN FRAGMENT
COMPND  12  RESIDUES 775 - 826
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   3 ORGANISM_COMMON: HUMAN;
SOURCE   4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE   5 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE   6 EXPRESSION_SYSTEM_PLASMID: PET28A(+);
SOURCE   7 MOL_ID: 2;
SOURCE   8 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   9 ORGANISM_COMMON: HUMAN;
SOURCE  10 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE  11 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE  12 EXPRESSION_SYSTEM_PLASMID: PGEX-GP-1
KEYWDS    FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
KEYWDS   2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
EXPDTA    X-RAY DIFFRACTION
AUTHOR    J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,I.SCHLEMMINGER,
AUTHOR   2 J.F.SEIBEL,C.J.SCHOFIELD
REVDAT   1   04-SEP-02 1H2M    0
JRNL        AUTH   J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,
JRNL        AUTH 2 I.SCHLEMMINGER,J.F.SEIBEL,C.J.SCHOFIELD
JRNL        TITL   FIH:HIF-FRAGMENT COMPLEXES
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK   2
REMARK   2 RESOLUTION. 2.5  ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.0
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) :   2.50
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) :  18.00
REMARK   3   DATA CUTOFF            (SIGMA(F)) : NONE
REMARK   3   COMPLETENESS FOR RANGE        (%) :  99.68
REMARK   3   NUMBER OF REFLECTIONS             :   18404
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
```

```
REMARK   3   CROSS-VALIDATION METHOD           : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION   : RANDOM
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.19432
REMARK   3   R VALUE            (WORKING SET) :  0.19185
REMARK   3   FREE R VALUE                      :  0.22491
REMARK   3   FREE R VALUE TEST SET SIZE   (%) :  7.6
REMARK   3   FREE R VALUE TEST SET COUNT       :  1516
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           :      20
REMARK   3   BIN RESOLUTION RANGE HIGH           :   2.500
REMARK   3   BIN RESOLUTION RANGE LOW            :   2.564
REMARK   3   REFLECTION IN BIN     (WORKING SET) :    1267
REMARK   3   BIN R VALUE           (WORKING SET) :   0.227
REMARK   3   BIN FREE R VALUE SET COUNT          :     106
REMARK   3   BIN FREE R VALUE                    :   0.297
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   ALL ATOMS                 :     2979
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) :  35.778
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :    -0.68
REMARK   3    B22 (A**2) :    -0.68
REMARK   3    B33 (A**2) :     1.35
REMARK   3    B12 (A**2) :     0.00
REMARK   3    B13 (A**2) :     0.00
REMARK   3    B23 (A**2) :     0.00
REMARK   3
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                                  (A):   0.334
REMARK   3   ESU BASED ON FREE R VALUE                             (A):   0.233
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                       (A):   0.224
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):   9.825
REMARK   3
REMARK   3 CORRELATION COEFFICIENTS.
REMARK   3   CORRELATION COEFFICIENT FO-FC      :   0.948
REMARK   3   CORRELATION COEFFICIENT FO-FC FREE :   0.935
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES         COUNT    RMS    WEIGHT
REMARK   3   BOND LENGTHS REFINED ATOMS        (A):  2957 ; 0.017 ; 0.021
REMARK   3   BOND LENGTHS OTHERS               (A):  2546 ; 0.001 ; 0.020
REMARK   3   BOND ANGLES REFINED ATOMS   (DEGREES):  4022 ; 1.612 ; 1.948
REMARK   3   BOND ANGLES OTHERS          (DEGREES):  5944 ; 0.832 ; 3.000
REMARK   3   TORSION ANGLES, PERIOD 1    (DEGREES):   350 ; 4.024 ; 3.000
REMARK   3   TORSION ANGLES, PERIOD 3    (DEGREES):   512 ;18.015 ;15.000
REMARK   3   CHIRAL-CENTER RESTRAINTS      (A**3):   413 ; 0.097 ; 0.200
REMARK   3   GENERAL PLANES REFINED ATOMS      (A):  3315 ; 0.006 ; 0.020
REMARK   3   GENERAL PLANES OTHERS             (A):   602 ; 0.002 ; 0.020
REMARK   3   NON-BONDED CONTACTS REFINED ATOMS (A):   731 ; 0.232 ; 0.300
REMARK   3   NON-BONDED CONTACTS OTHERS        (A):  2492 ; 0.214 ; 0.300
REMARK   3   H-BOND (X...Y) REFINED ATOMS      (A):   193 ; 0.173 ; 0.500
REMARK   3   H-BOND (X...Y) OTHERS             (A):     6 ; 0.126 ; 0.500
REMARK   3   POTENTIAL METAL-ION REFINED ATOMS (A):     2 ; 0.054 ; 0.500
REMARK   3   SYMMETRY VDW REFINED ATOMS        (A):    15 ; 0.194 ; 0.300
REMARK   3   SYMMETRY VDW OTHERS               (A):    54 ; 0.255 ; 0.300
REMARK   3   SYMMETRY H-BOND REFINED ATOMS     (A):     7 ; 0.244 ; 0.500
REMARK   3   SYMMETRY H-BOND OTHERS            (A):     1 ; 0.053 ; 0.500
REMARK   3
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REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.      COUNT   RMS     WEIGHT
REMARK   3   MAIN-CHAIN BOND REFINED ATOMS  (A**2):  1767 ; 0.761 ; 1.500
REMARK   3   MAIN-CHAIN ANGLE REFINED ATOMS (A**2):  2846 ; 1.421 ; 2.000
REMARK   3   SIDE-CHAIN BOND REFINED ATOMS  (A**2):  1190 ; 2.220 ; 3.000
REMARK   3   SIDE-CHAIN ANGLE REFINED ATOMS (A**2):  1176 ; 3.678 ; 4.500
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF NCS GROUPS : NULL
REMARK   3
REMARK   3  TLS DETAILS
REMARK   3   NUMBER OF TLS GROUPS  :    1
REMARK   3
REMARK   3   TLS GROUP :     1
REMARK   3    NUMBER OF COMPONENTS GROUP :    2
REMARK   3    COMPONENTS        C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :   A    15        A   451
REMARK   3    RESIDUE RANGE :   S   795        S   822
REMARK   3    ORIGIN FOR THE GROUP (A):  22.5990  26.9200  28.6340
REMARK   3    T TENSOR
REMARK   3      T11:   0.1903 T22:   0.0302
REMARK   3      T33:   0.0452 T12:  -0.0025
REMARK   3      T13:  -0.0536 T23:   0.0309
REMARK   3    L TENSOR
REMARK   3      L11:   0.7638 L22:   2.2674
REMARK   3      L33:   1.0629 L12:   0.7977
REMARK   3      L13:   0.4200 L23:   1.0769
REMARK   3    S TENSOR
REMARK   3      S11:   0.0306 S12:  -0.1225 S13:  -0.0490
REMARK   3      S21:   0.1656 S22:   0.0303 S23:   0.0478
REMARK   3      S31:   0.2046 S32:   0.0231 S33:  -0.0609
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED : BABINET MODEL WITH MASK
REMARK   3   PARAMETERS FOR MASK CALCULATION
REMARK   3   VDW PROBE RADIUS   :  1.40
REMARK   3   ION PROBE RADIUS   :  0.80
REMARK   3   SHRINKAGE RADIUS   :  0.80
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS:
REMARK   3  HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
REMARK   4
REMARK   4 1H2M COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI  ON 12-AUG-2002.
REMARK 100 THE EBI ID CODE IS EBI-11173.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : 15-MAY-2002
REMARK 200  TEMPERATURE           (KELVIN) : 100
REMARK 200  PH                             : 7.5
REMARK 200  NUMBER OF CRYSTALS USED        : 1
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : Y
REMARK 200  RADIATION SOURCE               : SRS BEAMLINE PX9.6
REMARK 200  BEAMLINE                       : PX9.6
REMARK 200  X-RAY GENERATOR MODEL          : NULL
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M
REMARK 200  WAVELENGTH OR RANGE        (A) : 0.87
REMARK 200  MONOCHROMATOR                  : NULL
REMARK 200  OPTICS                         : NULL
```

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REMARK 200
REMARK 200  DETECTOR TYPE                          : ADSC QUANTUM 4
REMARK 200  DETECTOR MANUFACTURER                  : ADSC
REMARK 200  INTENSITY-INTEGRATION SOFTWARE         : MOSFLM
REMARK 200  DATA SCALING SOFTWARE                  : SCALA
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS           : 20058
REMARK 200  RESOLUTION RANGE HIGH       (A)        : 2.50
REMARK 200  RESOLUTION RANGE LOW        (A)        : 87.71
REMARK 200  REJECTION CRITERIA  (SIGMA(I))         : NONE
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE      (%)        : 99.7
REMARK 200  DATA REDUNDANCY                        : 6.5
REMARK 200  R MERGE                     (I)        : 0.050
REMARK 200  R SYM                       (I)        : NULL
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET          : 10.7
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.50
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.64
REMARK 200  COMPLETENESS FOR SHELL      (%)        : 97.9
REMARK 200  DATA REDUNDANCY IN SHELL               : 4.4
REMARK 200  R MERGE FOR SHELL           (I)        : 0.289
REMARK 200  R SYM FOR SHELL             (I)        : NULL
REMARK 200  <I/SIGMA(I)> FOR SHELL                 : 2.6
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: NULL
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: NULL
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 63
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE,
REMARK 280  4% PEG400, 0.1M HEPES PH7.5, 11MG/ML PROTEIN WITH
REMARK 280  1MM FE(II), 2.5MM NOG AND 2.5MM PEPTIDE
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
REMARK 290       2555   -X,-Y,1/2+Z
REMARK 290       3555   1/2-Y,1/2+X,1/4+Z
REMARK 290       4555   1/2+Y,1/2-X,3/4+Z
REMARK 290       5555   1/2-X,1/2+Y,1/4-Z
REMARK 290       6555   1/2+X,1/2-Y,3/4-Z
REMARK 290       7555   Y,X,-Z
REMARK 290       8555   -Y,-X,1/2-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
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```
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000       74.13000
REMARK 290   SMTRY1   3  0.000000 -1.000000  0.000000       43.12450
REMARK 290   SMTRY2   3  1.000000  0.000000  0.000000       43.12450
REMARK 290   SMTRY3   3  0.000000  0.000000  1.000000       37.06500
REMARK 290   SMTRY1   4  0.000000  1.000000  0.000000       43.12450
REMARK 290   SMTRY2   4 -1.000000  0.000000  0.000000       43.12450
REMARK 290   SMTRY3   4  0.000000  0.000000  1.000000      111.19500
REMARK 290   SMTRY1   5 -1.000000  0.000000  0.000000       43.12450
REMARK 290   SMTRY2   5  0.000000  1.000000  0.000000       43.12450
REMARK 290   SMTRY3   5  0.000000  0.000000 -1.000000       37.06500
REMARK 290   SMTRY1   6  1.000000  0.000000  0.000000       43.12450
REMARK 290   SMTRY2   6  0.000000 -1.000000  0.000000       43.12450
REMARK 290   SMTRY3   6  0.000000  0.000000 -1.000000      111.19500
REMARK 290   SMTRY1   7  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY2   7  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY3   7  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   8  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY2   8 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY3   8  0.000000  0.000000 -1.000000       74.13000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF   2 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 300
REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: TETRAMERIC
REMARK 300
REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
REMARK 300 A HETERODIMERIC ASSOCIATION OF CHAIN A WITH CHAIN S
REMARK 300 PRODUCES A TETRAMER.
REMARK 300
REMARK 300 THE BURIED SURFACE AREA SHOWN BELOW IS AN AVERAGE
REMARK 300 CALCULATED FOR THE HETEROTETRAMER AND DOES NOT
REMARK 300 CORRESPOND TO THE BURIED SURFACE AREA FOR THE
REMARK 300 HOMODIMER OF CHAIN A
REMARK 300
REMARK 300 THE HETERO-ASSEMBLY DESCRIBED BY REMARK 350 APPEARS
REMARK 300 TO BE A CASE OF STRONG CRYSTAL PACKING WITH
REMARK 300 THE MEAN DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
REMARK 300 THE CHAIN IN THE COMPLEX IS     2149.4 ANGSTROM**2
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE:  1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, S
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000        0.00000
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```
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000        0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000        0.00000
REMARK 350   BIOMT1   2  0.000000 -1.000000  0.000000       86.24900
REMARK 350   BIOMT2   2 -1.000000  0.000000  0.000000       86.24900
REMARK 350   BIOMT3   2  0.000000  0.000000 -1.000000       74.13000
REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465     MET A     1
REMARK 465     ALA A     2
REMARK 465     ALA A     3
REMARK 465     THR A     4
REMARK 465     ALA A     5
REMARK 465     ALA A     6
REMARK 465     GLU A     7
REMARK 465     ALA A     8
REMARK 465     VAL A     9
REMARK 465     ALA A    10
REMARK 465     SER A    11
REMARK 465     GLY A    12
REMARK 465     SER A    13
REMARK 465     GLY A    14
REMARK 465     LYS A   304
REMARK 465     ARG A   305
REMARK 465     ILE A   306
REMARK 465     PRO S   775
REMARK 465     SER S   776
REMARK 465     ASP S   777
REMARK 465     LEU S   778
REMARK 465     ALA S   779
REMARK 465     CYS S   780
REMARK 465     ARG S   781
REMARK 465     LEU S   782
REMARK 465     LEU S   783
REMARK 465     GLY S   784
REMARK 465     GLN S   785
REMARK 465     SER S   786
REMARK 465     MET S   787
REMARK 465     ASP S   788
REMARK 465     GLU S   789
REMARK 465     SER S   790
REMARK 465     GLY S   791
REMARK 465     LEU S   792
REMARK 465     PRO S   793
REMARK 465     GLN S   794
REMARK 465     GLN S   807
REMARK 465     GLY S   808
REMARK 465     SER S   809
REMARK 465     ARG S   810
REMARK 465     ASN S   811
REMARK 465     LEU S   812
REMARK 465     ASP S   823
REMARK 465     GLN S   824
REMARK 465     VAL S   825
REMARK 465     ASN S   826
REMARK 470
REMARK 470 MISSING ATOM
```

```
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470   M RES CSSEQI  ATOMS
REMARK 470     GLU A  15    CG   CD   OE1  OE2
REMARK 470     GLU A  29    CG   CD   OE1  OE2
REMARK 470     ASN A  87    CG   OD1  ND2
REMARK 470     LYS A 106    CD   CE   NZ
REMARK 470     LYS A 115    CG   CD   CE   NZ
REMARK 470     ARG A 117    CG   CD   NE   CZ   NH1  NH2
REMARK 470     GLN A 133    CG   CD   OE1  NE2
REMARK 470     GLN A 136    CG   CD   OE1  NE2
REMARK 470     GLN A 137    CG   CD   OE1  NE2
REMARK 470     ARG A 156    CG   CD   NE   CZ   NH1  NH2
REMARK 470     LYS A 157    CD   CE   NZ
REMARK 470     LYS A 311    CG   CD   CE   NZ
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1   ATM2   ATM3
REMARK 500    LEU A 227   CA  -  CB  -  CG  ANGL. DEV. = -11.0 DEGREES
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 500 NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,1X,2(A4,A1,3X),12X,F5.3)
REMARK 500
REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1   RES CSSEQI ATM2   DEVIATION
REMARK 500    MET A 343  SD     MET A 343  CE      -0.209
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500  ATM1  RES C  SSEQI   ATM2  RES C  SSEQI          DISTANCE
REMARK 500
```

```
REMARK 500   O    ALA A   300     OH   TYR S   798              2.09
REMARK 525
REMARK 525 SOLVENT
REMARK 525
REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
REMARK 525 ASSOCIATED WITH:
REMARK 525   PROTEIN CHAIN  SOLVENT CHAIN
REMARK 525     A             Z
REMARK 525     S             H
REMARK 600
REMARK 600 HETEROGEN
REMARK 600
REMARK 600 FOR METAL ATOM ZN    ZN A1350  THE COORDINATION ANGLES ARE:
REMARK 600  1 HIS   199A  NE2
REMARK 600  2 ASP   201A  OD2       103.4
REMARK 600  3 HIS   279A  NE2        84.2  88.5
REMARK 600  4 OGA  1351A  O2        169.0  87.2  99.0
REMARK 600  5 OGA  1351A  O2'        86.3 169.1  97.3  82.8
REMARK 600                            1     2     3     4
REMARK 700
REMARK 700 SHEET
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
REMARK 700 TWO SHEETS ARE DEFINED.
REMARK 800
REMARK 800 SITE
REMARK 800 SITE_IDENTIFIER: ZNA
REMARK 800 SITE_DESCRIPTION: ZN BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: OGA
REMARK 800 SITE_DESCRIPTION: OGA BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: SA1
REMARK 800 SITE_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: SA2
REMARK 800 SITE_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1D7G   RELATED DB: PDB
REMARK 900  A MODEL FOR THE COMPLEX BETWEEN THE
REMARK 900  HYPOXIA-INDUCIBLE FACTOR-1 (HIF-1) AND ITS
REMARK 900   CONSENSUS DEOXYRIBONUCLEIC ACID SEQUENCE
REMARK 900 RELATED ID: 1H2K   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2L   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2N   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1L8C   RELATED DB: PDB
REMARK 900  STRUCTURAL BASIS FOR HIF-1ALPHA/CBP
REMARK 900  RECOGNITION IN THECELLULAR HYPOXIC RESPONSE
REMARK 900 RELATED ID: 1LM8   RELATED DB: PDB
REMARK 900  STRUCTURE OF A HIF-1A-PVHL-ELONGINB-
REMARK 900  ELONGINC COMPLEX
REMARK 900 RELATED ID: 1LQB   RELATED DB: PDB
REMARK 900  CRYSTAL STRUCTURE OF A HYDROXYLATED HIF-1
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REMARK 900  ALPHA PEPTIDEBOUND TO THE PVHL/ELONGIN-C/
REMARK 900  ELONGIN-B COMPLEX
DBREF  1H2M A    1   349  SWS    Q969Q7   Q969Q7             1    349
DBREF  1H2M S  775   826  SWS    Q16665   HIFA_HUMAN       775    826
SEQRES   1 A  349  MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
SEQRES   2 A  349  GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEQRES   3 A  349  TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
SEQRES   4 A  349  ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
SEQRES   5 A  349  GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
SEQRES   6 A  349  ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
SEQRES   7 A  349  GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
SEQRES   8 A  349  VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
SEQRES   9 A  349  GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
SEQRES  10 A  349  SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
SEQRES  11 A  349  LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
SEQRES  12 A  349  LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
SEQRES  13 A  349  LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP
SEQRES  14 A  349  ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
SEQRES  15 A  349  THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEQRES  16 A  349  THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA
SEQRES  17 A  349  GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
SEQRES  18 A  349  ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
SEQRES  19 A  349  PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
SEQRES  20 A  349  ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY
SEQRES  21 A  349  TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE
SEQRES  22 A  349  PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN
SEQRES  23 A  349  GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY
SEQRES  24 A  349  ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA
SEQRES  25 A  349  HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET
SEQRES  26 A  349  LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
SEQRES  27 A  349  LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
SEQRES   1 S   52  PRO SER ASP LEU ALA CYS ARG LEU LEU GLY GLN SER MET
SEQRES   2 S   52  ASP GLU SER GLY LEU PRO GLN LEU THR SER TYR ASP CYS
SEQRES   3 S   52  GLU VAL ASN ALA PRO ILE GLN GLY SER ARG ASN LEU LEU
SEQRES   4 S   52  GLN GLY GLU GLU LEU LEU ARG ALA LEU ASP GLN VAL ASN
HET     ZN  A1350       1
HET    OGA  A1351      10
HET    SO4  A1352       5
HET    SO4  A1353       5
HETNAM      ZN ZINC ION
HETNAM     OGA N-OXALYOLGLYCINE
HETNAM     SO4 SULFATE ION
FORMUL   3   ZN    ZN1 2+
FORMUL   4  OGA    C4 H5 N1 O5
FORMUL   5  SO4    2(O4 S1 2-)
FORMUL   6  HOH   *99(H2 O1)
HELIX    1   1 ASP A   28  LEU A   32  5                                   5
HELIX    2   2 ASP A   49  ASN A   58  1                                  10
HELIX    3   3 VAL A   70  TRP A   76  5                                   7
HELIX    4   4 ASP A   77  ILE A   85  1                                   9
HELIX    5   5 ASP A  104  GLN A  112  5                                   9
HELIX    6   6 LYS A  124  ARG A  138  1                                  15
HELIX    7   7 GLY A  155  GLY A  164  1                                  10
HELIX    8   8 ASN A  166  ARG A  177  1                                  12
HELIX    9   9 PRO A  220  ASP A  222  5                                   3
HELIX   10  10 GLN A  223  TYR A  228  1                                   6
HELIX   11  11 PHE A  252  VAL A  258  5                                   7
HELIX   12  12 LYS A  311  GLY A  331  1                                  21
HELIX   13  13 ASN A  332  GLN A  334  5                                   3
HELIX   14  14 GLU A  335  LYS A  345  1                                  11
HELIX   15  15 GLN S  814  LEU S  822  1                                   9
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SHEET    1  AA 5 THR A  39  PRO A  41  0
SHEET    2  AA 5 GLY A 260  VAL A 265  1  O  GLY A 260   N  ARG A  40
SHEET    3  AA 5 LYS A 214  PHE A 219 -1  O  LYS A 214   N  VAL A 265
SHEET    4  AA 5 TRP A 278  SER A 283 -1  O  TRP A 278   N  PHE A 219
SHEET    5  AA 5 VAL A 195  HIS A 199 -1  O  THR A 196   N  ILE A 281
SHEET    1  AB 6 ARG A  44  LEU A  45  0
SHEET    2  AB 6 VAL A  62  LEU A  64  1  O  VAL A  63   N  LEU A  45
SHEET    3  AB 6 VAL A 270  ILE A 273 -1  O  VAL A 270   N  LEU A  64
SHEET    4  AB 6 GLN A 203  LYS A 211 -1  O  ASN A 205   N  ILE A 273
SHEET    5  AB 6 THR A 290  LYS A 298 -1  O  ILE A 291   N  ILE A 210
SHEET    6  AB 6 LEU A 182  SER A 184 -1  N  THR A 183   O  TRP A 296
SHEET    1  AC 9 ARG A  44  LEU A  45  0
SHEET    2  AC 9 VAL A  62  LEU A  64  1  O  VAL A  63   N  LEU A  45
SHEET    3  AC 9 VAL A 270  ILE A 273 -1  O  VAL A 270   N  LEU A  64
SHEET    4  AC 9 GLN A 203  LYS A 211 -1  O  ASN A 205   N  ILE A 273
SHEET    5  AC 9 THR A 290  LYS A 298 -1  O  ILE A 291   N  ILE A 210
SHEET    6  AC 9 LEU A 186  GLY A 190 -1  O  LEU A 186   N  ASN A 294
SHEET    7  AC 9 ARG A 143  THR A 149 -1  O  LEU A 146   N  ILE A 189
SHEET    8  AC 9 PHE A  90  ALA A  95 -1  O  SER A  91   N  GLN A 147
SHEET    9  AC 9 SER A 118  MET A 123 -1  O  ASN A 119   N  SER A  94
LINK         ZN    ZN A1350                 NE2 HIS A 199     1555   1555
LINK         ZN    ZN A1350                 OD2 ASP A 201     1555   1555
LINK         ZN    ZN A1350                 NE2 HIS A 279     1555   1555
LINK         ZN    ZN A1350                 O2  OGA A1351     1555   1555
LINK         ZN    ZN A1350                 O2' OGA A1351     1555   1555
CISPEP   1 TYR A  308    PRO A  309          0         1.05
SITE     1 ZNA  3 HIS A 199  ASP A 201  HIS A 279
SITE     1 OGA 13 TYR A 145  LEU A 188  THR A 196  HIS A 199
SITE     2 OGA 13 ASP A 201  ASN A 205  PHE A 207  LYS A 214
SITE     3 OGA 13 HIS A 279  ILE A 281  ASN A 294  TRP A 296
SITE     4 OGA 13 HOH Z  47
SITE     1 SA1  4 ARG A 138  GLY A 140  GLU A 141  GLU A 142
SITE     1 SA2  5 ARG A 143  GLU A 192  GLY A 193  LEU A 285
SITE     2 SA2  5 ASN A 286
CRYST1   86.249   86.249  148.260  90.00  90.00  90.00 P 41 21 2     8
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.011594  0.000000  0.000000        0.00000
SCALE2      0.000000  0.011594  0.000000        0.00000
SCALE3      0.000000  0.000000  0.006745        0.00000
ATOM      1  N   GLU A  15       8.462  32.732   9.880  1.00 78.57           N
ATOM      2  CA  GLU A  15       7.114  32.108   9.773  1.00 78.75           C
ATOM      3  C   GLU A  15       7.207  30.654  10.192  1.00 78.42           C
ATOM      4  O   GLU A  15       8.067  29.928   9.714  1.00 78.63           O
ATOM      5  CB  GLU A  15       6.580  32.219   8.345  1.00 78.95           C
ATOM      6  N   PRO A  16       6.316  30.214  11.067  1.00 78.20           N
ATOM      7  CA  PRO A  16       6.376  28.840  11.584  1.00 77.89           C
ATOM      8  C   PRO A  16       6.328  27.796  10.467  1.00 77.35           C
ATOM      9  O   PRO A  16       5.541  27.888   9.527  1.00 76.95           O
ATOM     10  CB  PRO A  16       5.146  28.746  12.493  1.00 78.00           C
ATOM     11  CG  PRO A  16       4.763  30.167  12.790  1.00 78.28           C
ATOM     12  CD  PRO A  16       5.173  30.969  11.605  1.00 78.24           C
ATOM     13  N   ARG A  17       7.184  26.796  10.580  1.00 76.88           N
ATOM     14  CA  ARG A  17       7.264  25.749   9.575  1.00 76.63           C
ATOM     15  C   ARG A  17       6.005  24.891   9.539  1.00 75.45           C
ATOM     16  O   ARG A  17       5.247  24.836  10.505  1.00 75.40           O
ATOM     17  CB  ARG A  17       8.444  24.820   9.875  1.00 77.06           C
ATOM     18  CG  ARG A  17       9.816  25.481   9.900  1.00 78.68           C
ATOM     19  CD  ARG A  17      10.954  24.522  10.293  1.00 80.53           C
ATOM     20  NE  ARG A  17      10.908  24.086  11.699  1.00 82.60           N
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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 21 | CZ | ARG | A | 17 | 11.401 | 24.776 | 12.744 | 1.00 | 84.27 | C |
| ATOM | 22 | NH1 | ARG | A | 17 | 11.980 | 25.968 | 12.584 | 1.00 | 83.33 | N |
| ATOM | 23 | NH2 | ARG | A | 17 | 11.311 | 24.268 | 13.967 | 1.00 | 85.10 | N |
| ATOM | 24 | N | GLU | A | 18 | 5.796 | 24.209 | 8.421 | 1.00 | 74.01 | N |
| ATOM | 25 | CA | GLU | A | 18 | 4.692 | 23.274 | 8.319 | 1.00 | 72.99 | C |
| ATOM | 26 | C | GLU | A | 18 | 5.193 | 21.855 | 8.607 | 1.00 | 71.43 | C |
| ATOM | 27 | O | GLU | A | 18 | 6.210 | 21.421 | 8.061 | 1.00 | 70.71 | O |
| ATOM | 28 | CB | GLU | A | 18 | 4.033 | 23.352 | 6.938 | 1.00 | 73.29 | C |
| ATOM | 29 | CG | GLU | A | 18 | 3.333 | 24.677 | 6.659 | 1.00 | 73.91 | C |
| ATOM | 30 | CD | GLU | A | 18 | 1.949 | 24.794 | 7.283 | 1.00 | 74.30 | C |
| ATOM | 31 | OE1 | GLU | A | 18 | 1.355 | 23.776 | 7.692 | 1.00 | 74.07 | O |
| ATOM | 32 | OE2 | GLU | A | 18 | 1.444 | 25.929 | 7.356 | 1.00 | 75.76 | O |
| ATOM | 33 | N | GLU | A | 19 | 4.482 | 21.157 | 9.491 | 1.00 | 69.89 | N |
| ATOM | 34 | CA | GLU | A | 19 | 4.786 | 19.764 | 9.818 | 1.00 | 68.89 | C |
| ATOM | 35 | C | GLU | A | 19 | 4.393 | 18.854 | 8.661 | 1.00 | 66.65 | C |
| ATOM | 36 | O | GLU | A | 19 | 3.324 | 19.011 | 8.065 | 1.00 | 65.92 | O |
| ATOM | 37 | CB | GLU | A | 19 | 4.058 | 19.311 | 11.096 | 1.00 | 69.41 | C |
| ATOM | 38 | CG | GLU | A | 19 | 4.544 | 19.996 | 12.370 | 1.00 | 72.06 | C |
| ATOM | 39 | CD | GLU | A | 19 | 4.308 | 19.194 | 13.657 | 1.00 | 76.41 | C |
| ATOM | 40 | OE1 | GLU | A | 19 | 3.855 | 18.016 | 13.609 | 1.00 | 78.21 | O |
| ATOM | 41 | OE2 | GLU | A | 19 | 4.590 | 19.758 | 14.746 | 1.00 | 79.64 | O |
| ATOM | 42 | N | ALA | A | 20 | 5.283 | 17.919 | 8.349 | 1.00 | 64.54 | N |
| ATOM | 43 | CA | ALA | A | 20 | 5.067 | 16.921 | 7.303 | 1.00 | 63.03 | C |
| ATOM | 44 | C | ALA | A | 20 | 3.735 | 16.225 | 7.449 | 1.00 | 61.23 | C |
| ATOM | 45 | O | ALA | A | 20 | 3.303 | 15.903 | 8.556 | 1.00 | 60.61 | O |
| ATOM | 46 | CB | ALA | A | 20 | 6.177 | 15.889 | 7.312 | 1.00 | 62.82 | C |
| ATOM | 47 | N | GLY | A | 21 | 3.087 | 16.002 | 6.316 | 1.00 | 59.29 | N |
| ATOM | 48 | CA | GLY | A | 21 | 1.833 | 15.289 | 6.304 | 1.00 | 58.26 | C |
| ATOM | 49 | C | GLY | A | 21 | 0.651 | 16.200 | 6.530 | 1.00 | 57.44 | C |
| ATOM | 50 | O | GLY | A | 21 | -0.416 | 15.739 | 6.873 | 1.00 | 56.42 | O |
| ATOM | 51 | N | ALA | A | 22 | 0.858 | 17.500 | 6.341 | 1.00 | 57.28 | N |
| ATOM | 52 | CA | ALA | A | 22 | -0.182 | 18.509 | 6.492 | 1.00 | 56.92 | C |
| ATOM | 53 | C | ALA | A | 22 | -0.737 | 18.544 | 7.909 | 1.00 | 56.53 | C |
| ATOM | 54 | O | ALA | A | 22 | -1.926 | 18.737 | 8.108 | 1.00 | 56.32 | O |
| ATOM | 55 | CB | ALA | A | 22 | -1.285 | 18.277 | 5.488 | 1.00 | 57.10 | C |
| ATOM | 56 | N | LEU | A | 23 | 0.133 | 18.369 | 8.898 | 1.00 | 56.25 | N |
| ATOM | 57 | CA | LEU | A | 23 | -0.306 | 18.397 | 10.289 | 1.00 | 56.07 | C |
| ATOM | 58 | C | LEU | A | 23 | -0.385 | 19.811 | 10.827 | 1.00 | 55.03 | C |
| ATOM | 59 | O | LEU | A | 23 | -0.638 | 20.037 | 11.998 | 1.00 | 54.89 | O |
| ATOM | 60 | CB | LEU | A | 23 | 0.583 | 17.519 | 11.149 | 1.00 | 56.05 | C |
| ATOM | 61 | CG | LEU | A | 23 | 0.445 | 16.067 | 10.678 | 1.00 | 58.06 | C |
| ATOM | 62 | CD1 | LEU | A | 23 | 1.307 | 15.080 | 11.478 | 1.00 | 59.22 | C |
| ATOM | 63 | CD2 | LEU | A | 23 | -1.030 | 15.653 | 10.735 | 1.00 | 59.53 | C |
| ATOM | 64 | N | GLY | A | 24 | -0.202 | 20.768 | 9.941 | 1.00 | 54.17 | N |
| ATOM | 65 | CA | GLY | A | 24 | -0.337 | 22.151 | 10.305 | 1.00 | 53.43 | C |
| ATOM | 66 | C | GLY | A | 24 | 0.932 | 22.758 | 10.834 | 1.00 | 52.71 | C |
| ATOM | 67 | O | GLY | A | 24 | 2.025 | 22.189 | 10.807 | 1.00 | 52.28 | O |
| ATOM | 68 | N | PRO | A | 25 | 0.775 | 23.965 | 11.324 | 1.00 | 51.60 | N |
| ATOM | 69 | CA | PRO | A | 25 | 1.908 | 24.695 | 11.858 | 1.00 | 50.67 | C |
| ATOM | 70 | C | PRO | A | 25 | 2.310 | 24.047 | 13.168 | 1.00 | 49.52 | C |
| ATOM | 71 | O | PRO | A | 25 | 1.481 | 23.648 | 13.982 | 1.00 | 47.61 | O |
| ATOM | 72 | CB | PRO | A | 25 | 1.366 | 26.110 | 12.065 | 1.00 | 50.61 | C |
| ATOM | 73 | CG | PRO | A | 25 | -0.109 | 26.034 | 11.931 | 1.00 | 50.61 | C |
| ATOM | 74 | CD | PRO | A | 25 | -0.493 | 24.689 | 11.463 | 1.00 | 51.58 | C |
| ATOM | 75 | N | ALA | A | 26 | 3.616 | 23.922 | 13.321 | 1.00 | 49.47 | N |
| ATOM | 76 | CA | ALA | A | 26 | 4.218 | 23.390 | 14.526 | 1.00 | 49.29 | C |
| ATOM | 77 | C | ALA | A | 26 | 3.894 | 24.266 | 15.759 | 1.00 | 47.94 | C |
| ATOM | 78 | O | ALA | A | 26 | 3.646 | 23.735 | 16.836 | 1.00 | 48.27 | O |
| ATOM | 79 | CB | ALA | A | 26 | 5.712 | 23.288 | 14.328 | 1.00 | 49.68 | C |
| ATOM | 80 | N | TRP | A | 27 | 3.864 | 25.581 | 15.592 | 1.00 | 45.91 | N |
| ATOM | 81 | CA | TRP | A | 27 | 3.494 | 26.487 | 16.683 | 1.00 | 45.16 | C |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 82 | C | TRP | A | 27 | 3.003 | 27.818 | 16.107 | 1.00 | 44.47 | C |
| ATOM | 83 | O | TRP | A | 27 | 2.985 | 27.981 | 14.901 | 1.00 | 44.30 | O |
| ATOM | 84 | CB | TRP | A | 27 | 4.719 | 26.727 | 17.568 | 1.00 | 44.91 | C |
| ATOM | 85 | CG | TRP | A | 27 | 5.916 | 26.910 | 16.737 | 1.00 | 42.67 | C |
| ATOM | 86 | CD1 | TRP | A | 27 | 6.702 | 25.934 | 16.197 | 1.00 | 43.38 | C |
| ATOM | 87 | CD2 | TRP | A | 27 | 6.411 | 28.129 | 16.255 | 1.00 | 38.70 | C |
| ATOM | 88 | NE1 | TRP | A | 27 | 7.690 | 26.494 | 15.425 | 1.00 | 41.56 | N |
| ATOM | 89 | CE2 | TRP | A | 27 | 7.532 | 27.847 | 15.452 | 1.00 | 39.59 | C |
| ATOM | 90 | CE3 | TRP | A | 27 | 6.039 | 29.442 | 16.431 | 1.00 | 38.28 | C |
| ATOM | 91 | CZ2 | TRP | A | 27 | 8.284 | 28.827 | 14.861 | 1.00 | 39.74 | C |
| ATOM | 92 | CZ3 | TRP | A | 27 | 6.781 | 30.409 | 15.849 | 1.00 | 39.48 | C |
| ATOM | 93 | CH2 | TRP | A | 27 | 7.884 | 30.104 | 15.057 | 1.00 | 40.17 | C |
| ATOM | 94 | N | ASP | A | 28 | 2.580 | 28.760 | 16.941 | 1.00 | 43.91 | N |
| ATOM | 95 | CA | ASP | A | 28 | 2.230 | 30.079 | 16.417 | 1.00 | 43.87 | C |
| ATOM | 96 | C | ASP | A | 28 | 2.750 | 31.161 | 17.305 | 1.00 | 42.33 | C |
| ATOM | 97 | O | ASP | A | 28 | 3.191 | 30.901 | 18.409 | 1.00 | 42.11 | O |
| ATOM | 98 | CB | ASP | A | 28 | 0.722 | 30.251 | 16.199 | 1.00 | 44.82 | C |
| ATOM | 99 | CG | ASP | A | 28 | -0.052 | 30.162 | 17.462 | 1.00 | 47.87 | C |
| ATOM | 100 | OD1 | ASP | A | 28 | -0.240 | 31.236 | 18.108 | 1.00 | 50.91 | O |
| ATOM | 101 | OD2 | ASP | A | 28 | -0.501 | 29.054 | 17.877 | 1.00 | 49.06 | O |
| ATOM | 102 | N | GLU | A | 29 | 2.713 | 32.385 | 16.790 | 1.00 | 41.29 | N |
| ATOM | 103 | CA | GLU | A | 29 | 3.208 | 33.586 | 17.499 | 1.00 | 39.69 | C |
| ATOM | 104 | C | GLU | A | 29 | 2.685 | 33.711 | 18.917 | 1.00 | 37.94 | C |
| ATOM | 105 | O | GLU | A | 29 | 3.415 | 34.069 | 19.801 | 1.00 | 37.26 | O |
| ATOM | 106 | CB | GLU | A | 29 | 2.840 | 34.812 | 16.735 | 1.00 | 39.59 | C |
| ATOM | 107 | N | SER | A | 30 | 1.427 | 33.371 | 19.135 | 1.00 | 36.78 | N |
| ATOM | 108 | CA | SER | A | 30 | 0.810 | 33.558 | 20.443 | 1.00 | 36.13 | C |
| ATOM | 109 | C | SER | A | 30 | 1.501 | 32.756 | 21.517 | 1.00 | 35.30 | C |
| ATOM | 110 | O | SER | A | 30 | 1.252 | 32.968 | 22.678 | 1.00 | 35.21 | O |
| ATOM | 111 | CB | SER | A | 30 | -0.686 | 33.180 | 20.406 | 1.00 | 35.84 | C |
| ATOM | 112 | OG | SER | A | 30 | -0.901 | 31.762 | 20.450 | 1.00 | 36.93 | O |
| ATOM | 113 | N | GLN | A | 31 | 2.326 | 31.795 | 21.116 | 1.00 | 35.24 | N |
| ATOM | 114 | CA | GLN | A | 31 | 3.021 | 30.918 | 22.060 | 1.00 | 34.89 | C |
| ATOM | 115 | C | GLN | A | 31 | 4.366 | 31.506 | 22.487 | 1.00 | 34.60 | C |
| ATOM | 116 | O | GLN | A | 31 | 5.010 | 30.969 | 23.365 | 1.00 | 34.18 | O |
| ATOM | 117 | CB | GLN | A | 31 | 3.224 | 29.513 | 21.473 | 1.00 | 34.65 | C |
| ATOM | 118 | CG | GLN | A | 31 | 1.969 | 28.649 | 21.402 | 1.00 | 34.74 | C |
| ATOM | 119 | CD | GLN | A | 31 | 2.212 | 27.322 | 20.707 | 1.00 | 33.47 | C |
| ATOM | 120 | OE1 | GLN | A | 31 | 2.215 | 27.249 | 19.476 | 1.00 | 32.57 | O |
| ATOM | 121 | NE2 | GLN | A | 31 | 2.442 | 26.278 | 21.492 | 1.00 | 32.95 | N |
| ATOM | 122 | N | LEU | A | 32 | 4.753 | 32.632 | 21.895 | 1.00 | 34.85 | N |
| ATOM | 123 | CA | LEU | A | 32 | 6.016 | 33.293 | 22.212 | 1.00 | 35.01 | C |
| ATOM | 124 | C | LEU | A | 32 | 5.798 | 34.391 | 23.223 | 1.00 | 34.91 | C |
| ATOM | 125 | O | LEU | A | 32 | 4.834 | 35.134 | 23.125 | 1.00 | 35.83 | O |
| ATOM | 126 | CB | LEU | A | 32 | 6.631 | 33.885 | 20.945 | 1.00 | 34.96 | C |
| ATOM | 127 | CG | LEU | A | 32 | 6.995 | 32.860 | 19.849 | 1.00 | 36.03 | C |
| ATOM | 128 | CD1 | LEU | A | 32 | 7.691 | 33.525 | 18.701 | 1.00 | 36.15 | C |
| ATOM | 129 | CD2 | LEU | A | 32 | 7.855 | 31.780 | 20.377 | 1.00 | 35.18 | C |
| ATOM | 130 | N | ARG | A | 33 | 6.675 | 34.500 | 24.209 | 1.00 | 34.49 | N |
| ATOM | 131 | CA | ARG | A | 33 | 6.564 | 35.591 | 25.170 | 1.00 | 34.33 | C |
| ATOM | 132 | C | ARG | A | 33 | 7.005 | 36.867 | 24.460 | 1.00 | 34.37 | C |
| ATOM | 133 | O | ARG | A | 33 | 7.733 | 36.815 | 23.498 | 1.00 | 34.87 | O |
| ATOM | 134 | CB | ARG | A | 33 | 7.442 | 35.338 | 26.394 | 1.00 | 34.16 | C |
| ATOM | 135 | CG | ARG | A | 33 | 7.056 | 34.124 | 27.212 | 1.00 | 32.83 | C |
| ATOM | 136 | CD | ARG | A | 33 | 7.951 | 33.894 | 28.428 | 1.00 | 33.34 | C |
| ATOM | 137 | NE | ARG | A | 33 | 7.413 | 32.820 | 29.252 | 1.00 | 34.91 | N |
| ATOM | 138 | CZ | ARG | A | 33 | 6.445 | 32.963 | 30.137 | 1.00 | 36.53 | C |
| ATOM | 139 | NH1 | ARG | A | 33 | 5.900 | 34.144 | 30.382 | 1.00 | 34.89 | N |
| ATOM | 140 | NH2 | ARG | A | 33 | 6.027 | 31.905 | 30.795 | 1.00 | 39.39 | N |
| ATOM | 141 | N | SER | A | 34 | 6.608 | 38.022 | 24.947 | 1.00 | 34.36 | N |
| ATOM | 142 | CA | SER | A | 34 | 6.944 | 39.247 | 24.244 | 1.00 | 34.69 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 143 | C | SER | A | 34 | 8.002 | 40.055 | 24.987 | 1.00 | 33.26 | C |
| ATOM | 144 | O | SER | A | 34 | 7.958 | 40.142 | 26.200 | 1.00 | 33.50 | O |
| ATOM | 145 | CB | SER | A | 34 | 5.698 | 40.096 | 24.143 | 1.00 | 35.23 | C |
| ATOM | 146 | OG | SER | A | 34 | 5.586 | 40.744 | 25.393 | 1.00 | 39.99 | O |
| ATOM | 147 | N | TYR | A | 35 | 8.911 | 40.682 | 24.252 | 1.00 | 32.38 | N |
| ATOM | 148 | CA | TYR | A | 35 | 10.080 | 41.329 | 24.843 | 1.00 | 32.03 | C |
| ATOM | 149 | C | TYR | A | 35 | 10.339 | 42.675 | 24.193 | 1.00 | 32.52 | C |
| ATOM | 150 | O | TYR | A | 35 | 9.763 | 42.979 | 23.172 | 1.00 | 32.78 | O |
| ATOM | 151 | CB | TYR | A | 35 | 11.290 | 40.422 | 24.686 | 1.00 | 31.20 | C |
| ATOM | 152 | CG | TYR | A | 35 | 11.139 | 39.161 | 25.482 | 1.00 | 30.69 | C |
| ATOM | 153 | CD1 | TYR | A | 35 | 10.935 | 39.215 | 26.853 | 1.00 | 30.40 | C |
| ATOM | 154 | CD2 | TYR | A | 35 | 11.186 | 37.915 | 24.875 | 1.00 | 30.34 | C |
| ATOM | 155 | CE1 | TYR | A | 35 | 10.804 | 38.054 | 27.609 | 1.00 | 31.74 | C |
| ATOM | 156 | CE2 | TYR | A | 35 | 11.050 | 36.741 | 25.617 | 1.00 | 32.05 | C |
| ATOM | 157 | CZ | TYR | A | 35 | 10.858 | 36.812 | 26.991 | 1.00 | 31.98 | C |
| ATOM | 158 | OH | TYR | A | 35 | 10.687 | 35.658 | 27.742 | 1.00 | 30.13 | O |
| ATOM | 159 | N | SER | A | 36 | 11.240 | 43.463 | 24.761 | 1.00 | 33.06 | N |
| ATOM | 160 | CA | SER | A | 36 | 11.469 | 44.838 | 24.289 | 1.00 | 32.95 | C |
| ATOM | 161 | C | SER | A | 36 | 12.469 | 44.977 | 23.159 | 1.00 | 32.65 | C |
| ATOM | 162 | O | SER | A | 36 | 12.705 | 46.084 | 22.674 | 1.00 | 33.04 | O |
| ATOM | 163 | CB | SER | A | 36 | 11.979 | 45.698 | 25.438 | 1.00 | 32.92 | C |
| ATOM | 164 | OG | SER | A | 36 | 13.272 | 45.325 | 25.844 | 1.00 | 33.05 | O |
| ATOM | 165 | N | PHE | A | 37 | 13.041 | 43.880 | 22.711 | 1.00 | 31.44 | N |
| ATOM | 166 | CA | PHE | A | 37 | 14.100 | 43.988 | 21.740 | 1.00 | 31.55 | C |
| ATOM | 167 | C | PHE | A | 37 | 13.784 | 43.269 | 20.444 | 1.00 | 31.69 | C |
| ATOM | 168 | O | PHE | A | 37 | 13.020 | 42.326 | 20.386 | 1.00 | 32.65 | O |
| ATOM | 169 | CB | PHE | A | 37 | 15.421 | 43.431 | 22.339 | 1.00 | 30.68 | C |
| ATOM | 170 | CG | PHE | A | 37 | 15.275 | 42.054 | 22.890 | 1.00 | 30.10 | C |
| ATOM | 171 | CD1 | PHE | A | 37 | 15.329 | 40.967 | 22.060 | 1.00 | 28.43 | C |
| ATOM | 172 | CD2 | PHE | A | 37 | 15.022 | 41.852 | 24.231 | 1.00 | 29.43 | C |
| ATOM | 173 | CE1 | PHE | A | 37 | 15.168 | 39.679 | 22.564 | 1.00 | 31.59 | C |
| ATOM | 174 | CE2 | PHE | A | 37 | 14.852 | 40.580 | 24.733 | 1.00 | 30.52 | C |
| ATOM | 175 | CZ | PHE | A | 37 | 14.927 | 39.495 | 23.915 | 1.00 | 31.81 | C |
| ATOM | 176 | N | PRO | A | 38 | 14.403 | 43.721 | 19.384 | 1.00 | 31.70 | N |
| ATOM | 177 | CA | PRO | A | 38 | 14.268 | 43.036 | 18.106 | 1.00 | 31.23 | C |
| ATOM | 178 | C | PRO | A | 38 | 15.231 | 41.895 | 17.984 | 1.00 | 31.71 | C |
| ATOM | 179 | O | PRO | A | 38 | 16.205 | 41.880 | 18.743 | 1.00 | 31.59 | O |
| ATOM | 180 | CB | PRO | A | 38 | 14.652 | 44.118 | 17.117 | 1.00 | 31.44 | C |
| ATOM | 181 | CG | PRO | A | 38 | 15.636 | 45.005 | 17.922 | 1.00 | 32.43 | C |
| ATOM | 182 | CD | PRO | A | 38 | 15.186 | 44.973 | 19.320 | 1.00 | 30.26 | C |
| ATOM | 183 | N | THR | A | 39 | 14.996 | 41.008 | 17.003 | 1.00 | 31.90 | N |
| ATOM | 184 | CA | THR | A | 39 | 15.868 | 39.891 | 16.702 | 1.00 | 32.00 | C |
| ATOM | 185 | C | THR | A | 39 | 15.865 | 39.606 | 15.203 | 1.00 | 32.89 | C |
| ATOM | 186 | O | THR | A | 39 | 14.998 | 40.048 | 14.476 | 1.00 | 32.28 | O |
| ATOM | 187 | CB | THR | A | 39 | 15.370 | 38.647 | 17.377 | 1.00 | 32.26 | C |
| ATOM | 188 | OG1 | THR | A | 39 | 14.024 | 38.389 | 16.949 | 1.00 | 30.59 | O |
| ATOM | 189 | CG2 | THR | A | 39 | 15.235 | 38.832 | 18.905 | 1.00 | 32.99 | C |
| ATOM | 190 | N | ARG | A | 40 | 16.855 | 38.844 | 14.770 | 1.00 | 33.28 | N |
| ATOM | 191 | CA | ARG | A | 40 | 16.980 | 38.372 | 13.421 | 1.00 | 34.30 | C |
| ATOM | 192 | C | ARG | A | 40 | 17.023 | 36.853 | 13.562 | 1.00 | 33.77 | C |
| ATOM | 193 | O | ARG | A | 40 | 17.288 | 36.324 | 14.614 | 1.00 | 34.68 | O |
| ATOM | 194 | CB | ARG | A | 40 | 18.267 | 38.847 | 12.795 | 1.00 | 34.73 | C |
| ATOM | 195 | CG | ARG | A | 40 | 18.273 | 40.306 | 12.451 | 1.00 | 41.24 | C |
| ATOM | 196 | CD | ARG | A | 40 | 16.909 | 40.799 | 12.022 | 1.00 | 48.38 | C |
| ATOM | 197 | NE | ARG | A | 40 | 16.728 | 41.025 | 10.597 | 1.00 | 51.83 | N |
| ATOM | 198 | CZ | ARG | A | 40 | 15.553 | 41.291 | 10.092 | 1.00 | 56.70 | C |
| ATOM | 199 | NH1 | ARG | A | 40 | 14.501 | 41.300 | 10.908 | 1.00 | 57.84 | N |
| ATOM | 200 | NH2 | ARG | A | 40 | 15.415 | 41.549 | 8.795 | 1.00 | 60.30 | N |
| ATOM | 201 | N | PRO | A | 41 | 16.663 | 36.147 | 12.533 | 1.00 | 33.50 | N |
| ATOM | 202 | CA | PRO | A | 41 | 16.646 | 34.681 | 12.569 | 1.00 | 33.48 | C |
| ATOM | 203 | C | PRO | A | 41 | 18.002 | 34.010 | 12.475 | 1.00 | 32.72 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 204 | O | PRO | A | 41 | 18.907 | 34.475 | 11.801 | 1.00 | 34.64 | O |
| ATOM | 205 | CB | PRO | A | 41 | 15.800 | 34.299 | 11.340 | 1.00 | 33.22 | C |
| ATOM | 206 | CG | PRO | A | 41 | 15.409 | 35.563 | 10.675 | 1.00 | 33.55 | C |
| ATOM | 207 | CD | PRO | A | 41 | 16.038 | 36.717 | 11.343 | 1.00 | 32.95 | C |
| ATOM | 208 | N | ILE | A | 42 | 18.154 | 32.925 | 13.192 | 1.00 | 30.97 | N |
| ATOM | 209 | CA | ILE | A | 42 | 19.337 | 32.144 | 13.049 | 1.00 | 29.87 | C |
| ATOM | 210 | C | ILE | A | 42 | 19.077 | 31.289 | 11.814 | 1.00 | 30.07 | C |
| ATOM | 211 | O | ILE | A | 42 | 17.946 | 30.857 | 11.587 | 1.00 | 30.17 | O |
| ATOM | 212 | CB | ILE | A | 42 | 19.477 | 31.306 | 14.273 | 1.00 | 29.85 | C |
| ATOM | 213 | CG1 | ILE | A | 42 | 19.721 | 32.215 | 15.478 | 1.00 | 27.79 | C |
| ATOM | 214 | CG2 | ILE | A | 42 | 20.582 | 30.264 | 14.105 | 1.00 | 30.60 | C |
| ATOM | 215 | CD1 | ILE | A | 42 | 19.565 | 31.503 | 16.788 | 1.00 | 25.35 | C |
| ATOM | 216 | N | PRO | A | 43 | 20.085 | 31.075 | 10.985 | 1.00 | 29.34 | N |
| ATOM | 217 | CA | PRO | A | 43 | 19.922 | 30.219 | 9.823 | 1.00 | 29.60 | C |
| ATOM | 218 | C | PRO | A | 43 | 19.623 | 28.751 | 10.176 | 1.00 | 30.65 | C |
| ATOM | 219 | O | PRO | A | 43 | 20.207 | 28.265 | 11.160 | 1.00 | 31.73 | O |
| ATOM | 220 | CB | PRO | A | 43 | 21.288 | 30.310 | 9.139 | 1.00 | 30.00 | C |
| ATOM | 221 | CG | PRO | A | 43 | 21.933 | 31.491 | 9.665 | 1.00 | 28.87 | C |
| ATOM | 222 | CD | PRO | A | 43 | 21.420 | 31.676 | 11.047 | 1.00 | 28.76 | C |
| ATOM | 223 | N | ARG | A | 44 | 18.725 | 28.103 | 9.419 | 1.00 | 30.34 | N |
| ATOM | 224 | CA | ARG | A | 44 | 18.415 | 26.693 | 9.507 | 1.00 | 31.59 | C |
| ATOM | 225 | C | ARG | A | 44 | 18.965 | 26.050 | 8.267 | 1.00 | 31.44 | C |
| ATOM | 226 | O | ARG | A | 44 | 18.540 | 26.359 | 7.169 | 1.00 | 32.24 | O |
| ATOM | 227 | CB | ARG | A | 44 | 16.923 | 26.399 | 9.502 | 1.00 | 32.07 | C |
| ATOM | 228 | CG | ARG | A | 44 | 16.105 | 27.115 | 10.563 | 1.00 | 36.61 | C |
| ATOM | 229 | CD | ARG | A | 44 | 14.638 | 26.534 | 10.809 | 1.00 | 39.09 | C |
| ATOM | 230 | NE | ARG | A | 44 | 14.350 | 25.140 | 10.395 | 1.00 | 41.98 | N |
| ATOM | 231 | CZ | ARG | A | 44 | 14.179 | 24.099 | 11.246 | 1.00 | 43.25 | C |
| ATOM | 232 | NH1 | ARG | A | 44 | 14.332 | 24.244 | 12.561 | 1.00 | 40.76 | N |
| ATOM | 233 | NH2 | ARG | A | 44 | 13.864 | 22.892 | 10.777 | 1.00 | 44.70 | N |
| ATOM | 234 | N | LEU | A | 45 | 19.878 | 25.118 | 8.428 | 1.00 | 31.29 | N |
| ATOM | 235 | CA | LEU | A | 45 | 20.544 | 24.560 | 7.294 | 1.00 | 30.82 | C |
| ATOM | 236 | C | LEU | A | 45 | 20.744 | 23.083 | 7.470 | 1.00 | 31.52 | C |
| ATOM | 237 | O | LEU | A | 45 | 20.690 | 22.550 | 8.597 | 1.00 | 31.99 | O |
| ATOM | 238 | CB | LEU | A | 45 | 21.909 | 25.221 | 7.134 | 1.00 | 29.63 | C |
| ATOM | 239 | CG | LEU | A | 45 | 21.873 | 26.697 | 6.813 | 1.00 | 31.00 | C |
| ATOM | 240 | CD1 | LEU | A | 45 | 23.279 | 27.338 | 7.030 | 1.00 | 31.79 | C |
| ATOM | 241 | CD2 | LEU | A | 45 | 21.403 | 26.918 | 5.378 | 1.00 | 31.14 | C |
| ATOM | 242 | N | SER | A | 46 | 21.004 | 22.437 | 6.338 | 1.00 | 31.72 | N |
| ATOM | 243 | CA | SER | A | 46 | 21.345 | 21.057 | 6.327 | 1.00 | 32.17 | C |
| ATOM | 244 | C | SER | A | 46 | 22.771 | 20.978 | 6.767 | 1.00 | 32.55 | C |
| ATOM | 245 | O | SER | A | 46 | 23.568 | 21.871 | 6.562 | 1.00 | 31.31 | O |
| ATOM | 246 | CB | SER | A | 46 | 21.255 | 20.447 | 4.936 | 1.00 | 32.06 | C |
| ATOM | 247 | OG | SER | A | 46 | 21.909 | 19.187 | 4.931 | 1.00 | 31.15 | O |
| ATOM | 248 | N | GLN | A | 47 | 23.068 | 19.849 | 7.358 | 1.00 | 33.60 | N |
| ATOM | 249 | CA | GLN | A | 47 | 24.370 | 19.546 | 7.878 | 1.00 | 34.42 | C |
| ATOM | 250 | C | GLN | A | 47 | 25.385 | 19.453 | 6.754 | 1.00 | 34.74 | C |
| ATOM | 251 | O | GLN | A | 47 | 26.554 | 19.685 | 6.971 | 1.00 | 35.40 | O |
| ATOM | 252 | CB | GLN | A | 47 | 24.232 | 18.194 | 8.593 | 1.00 | 35.09 | C |
| ATOM | 253 | CG | GLN | A | 47 | 25.465 | 17.417 | 8.733 | 1.00 | 36.19 | C |
| ATOM | 254 | CD | GLN | A | 47 | 25.670 | 16.422 | 7.678 | 1.00 | 36.93 | C |
| ATOM | 255 | OE1 | GLN | A | 47 | 24.757 | 16.093 | 6.902 | 1.00 | 38.75 | O |
| ATOM | 256 | NE2 | GLN | A | 47 | 26.894 | 15.903 | 7.630 | 1.00 | 40.53 | N |
| ATOM | 257 | N | SER | A | 48 | 24.933 | 19.095 | 5.556 | 1.00 | 34.63 | N |
| ATOM | 258 | CA | SER | A | 48 | 25.821 | 18.922 | 4.415 | 1.00 | 34.93 | C |
| ATOM | 259 | C | SER | A | 48 | 26.128 | 20.249 | 3.735 | 1.00 | 35.90 | C |
| ATOM | 260 | O | SER | A | 48 | 26.990 | 20.315 | 2.862 | 1.00 | 36.31 | O |
| ATOM | 261 | CB | SER | A | 48 | 25.182 | 17.991 | 3.381 | 1.00 | 34.59 | C |
| ATOM | 262 | OG | SER | A | 48 | 23.912 | 18.483 | 2.955 | 1.00 | 33.48 | O |
| ATOM | 263 | N | ASP | A | 49 | 25.415 | 21.302 | 4.124 | 1.00 | 36.41 | N |
| ATOM | 264 | CA | ASP | A | 49 | 25.583 | 22.606 | 3.512 | 1.00 | 37.09 | C |

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ATOM    265  C   ASP A  49      26.855  23.291   3.989  1.00 37.81           C
ATOM    266  O   ASP A  49      27.020  23.523   5.182  1.00 36.99           O
ATOM    267  CB  ASP A  49      24.383  23.451   3.877  1.00 37.42           C
ATOM    268  CG  ASP A  49      24.323  24.733   3.117  1.00 38.29           C
ATOM    269  OD1 ASP A  49      25.383  25.351   2.849  1.00 37.80           O
ATOM    270  OD2 ASP A  49      23.223  25.191   2.760  1.00 40.61           O
ATOM    271  N   PRO A  50      27.740  23.649   3.056  1.00 38.39           N
ATOM    272  CA  PRO A  50      29.005  24.291   3.409  1.00 38.24           C
ATOM    273  C   PRO A  50      28.802  25.502   4.285  1.00 38.16           C
ATOM    274  O   PRO A  50      29.671  25.797   5.088  1.00 37.37           O
ATOM    275  CB  PRO A  50      29.577  24.738   2.051  1.00 38.14           C
ATOM    276  CG  PRO A  50      28.978  23.915   1.070  1.00 38.31           C
ATOM    277  CD  PRO A  50      27.620  23.473   1.601  1.00 38.85           C
ATOM    278  N   ARG A  51      27.686  26.199   4.125  1.00 38.66           N
ATOM    279  CA  ARG A  51      27.448  27.403   4.912  1.00 39.05           C
ATOM    280  C   ARG A  51      27.332  27.077   6.391  1.00 38.94           C
ATOM    281  O   ARG A  51      27.668  27.908   7.259  1.00 38.35           O
ATOM    282  CB  ARG A  51      26.199  28.120   4.438  1.00 39.34           C
ATOM    283  CG  ARG A  51      26.372  28.781   3.067  1.00 41.10           C
ATOM    284  CD  ARG A  51      25.099  29.355   2.486  1.00 42.20           C
ATOM    285  NE  ARG A  51      24.111  28.314   2.192  1.00 44.96           N
ATOM    286  CZ  ARG A  51      22.815  28.551   2.043  1.00 46.68           C
ATOM    287  NH1 ARG A  51      22.348  29.795   2.162  1.00 47.61           N
ATOM    288  NH2 ARG A  51      21.980  27.563   1.774  1.00 46.08           N
ATOM    289  N   ALA A  52      26.882  25.867   6.688  1.00 38.31           N
ATOM    290  CA  ALA A  52      26.729  25.498   8.082  1.00 38.63           C
ATOM    291  C   ALA A  52      28.093  25.311   8.677  1.00 38.81           C
ATOM    292  O   ALA A  52      28.341  25.682   9.816  1.00 39.03           O
ATOM    293  CB  ALA A  52      25.907  24.233   8.235  1.00 38.36           C
ATOM    294  N   GLU A  53      28.988  24.733   7.899  1.00 39.48           N
ATOM    295  CA  GLU A  53      30.316  24.484   8.388  1.00 40.51           C
ATOM    296  C   GLU A  53      31.038  25.802   8.621  1.00 40.41           C
ATOM    297  O   GLU A  53      31.740  25.954   9.618  1.00 39.82           O
ATOM    298  CB  GLU A  53      31.093  23.614   7.436  1.00 40.70           C
ATOM    299  CG  GLU A  53      32.129  22.790   8.171  1.00 44.79           C
ATOM    300  CD  GLU A  53      31.596  21.435   8.633  1.00 48.98           C
ATOM    301  OE1 GLU A  53      30.427  21.329   9.017  1.00 51.56           O
ATOM    302  OE2 GLU A  53      32.354  20.454   8.620  1.00 54.44           O
ATOM    303  N   GLU A  54      30.851  26.752   7.713  1.00 40.45           N
ATOM    304  CA  GLU A  54      31.465  28.060   7.853  1.00 41.40           C
ATOM    305  C   GLU A  54      30.991  28.731   9.162  1.00 40.32           C
ATOM    306  O   GLU A  54      31.760  29.374   9.836  1.00 39.89           O
ATOM    307  CB  GLU A  54      31.119  28.974   6.679  1.00 42.12           C
ATOM    308  CG  GLU A  54      31.697  28.557   5.333  1.00 47.25           C
ATOM    309  CD  GLU A  54      30.953  29.191   4.129  1.00 53.54           C
ATOM    310  OE1 GLU A  54      30.459  30.366   4.276  1.00 57.47           O
ATOM    311  OE2 GLU A  54      30.882  28.527   3.036  1.00 53.82           O
ATOM    312  N   LEU A  55      29.735  28.534   9.533  1.00 39.03           N
ATOM    313  CA  LEU A  55      29.223  29.198  10.687  1.00 37.80           C
ATOM    314  C   LEU A  55      29.840  28.673  11.956  1.00 36.83           C
ATOM    315  O   LEU A  55      30.293  29.464  12.795  1.00 35.66           O
ATOM    316  CB  LEU A  55      27.715  29.081  10.725  1.00 38.06           C
ATOM    317  CG  LEU A  55      27.072  29.921   9.621  1.00 37.63           C
ATOM    318  CD1 LEU A  55      25.620  29.569   9.449  1.00 39.63           C
ATOM    319  CD2 LEU A  55      27.174  31.356   9.928  1.00 36.27           C
ATOM    320  N   ILE A  56      29.876  27.346  12.079  1.00 35.87           N
ATOM    321  CA  ILE A  56      30.436  26.684  13.257  1.00 35.35           C
ATOM    322  C   ILE A  56      31.916  27.001  13.410  1.00 35.82           C
ATOM    323  O   ILE A  56      32.377  27.299  14.499  1.00 36.59           O
ATOM    324  CB  ILE A  56      30.281  25.198  13.139  1.00 34.84           C
ATOM    325  CG1 ILE A  56      28.790  24.810  13.132  1.00 34.00           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 326 | CG2 | ILE | A | 56 | 31.022 | 24.535 | 14.280 | 1.00 | 34.89 | C |
| ATOM | 327 | CD1 | ILE | A | 56 | 28.502 | 23.361 | 12.684 | 1.00 | 30.65 | C |
| ATOM | 328 | N | GLU | A | 57 | 32.636 | 26.964 | 12.301 | 1.00 | 36.28 | N |
| ATOM | 329 | CA | GLU | A | 57 | 34.056 | 27.244 | 12.255 | 1.00 | 37.26 | C |
| ATOM | 330 | C | GLU | A | 57 | 34.295 | 28.634 | 12.809 | 1.00 | 37.41 | C |
| ATOM | 331 | O | GLU | A | 57 | 35.278 | 28.879 | 13.516 | 1.00 | 38.73 | O |
| ATOM | 332 | CB | GLU | A | 57 | 34.562 | 27.167 | 10.795 | 1.00 | 37.54 | C |
| ATOM | 333 | CG | GLU | A | 57 | 36.035 | 27.462 | 10.572 | 1.00 | 39.41 | C |
| ATOM | 334 | CD | GLU | A | 57 | 36.948 | 26.668 | 11.493 | 1.00 | 44.86 | C |
| ATOM | 335 | OE1 | GLU | A | 57 | 36.666 | 25.458 | 11.741 | 1.00 | 48.72 | O |
| ATOM | 336 | OE2 | GLU | A | 57 | 37.961 | 27.260 | 11.965 | 1.00 | 46.32 | O |
| ATOM | 337 | N | ASN | A | 58 | 33.386 | 29.537 | 12.485 | 1.00 | 36.64 | N |
| ATOM | 338 | CA | ASN | A | 58 | 33.456 | 30.907 | 12.926 | 1.00 | 36.26 | C |
| ATOM | 339 | C | ASN | A | 58 | 32.768 | 31.226 | 14.219 | 1.00 | 35.28 | C |
| ATOM | 340 | O | ASN | A | 58 | 32.569 | 32.376 | 14.531 | 1.00 | 33.45 | O |
| ATOM | 341 | CB | ASN | A | 58 | 32.798 | 31.758 | 11.898 | 1.00 | 36.88 | C |
| ATOM | 342 | CG | ASN | A | 58 | 33.763 | 32.461 | 11.107 | 1.00 | 39.77 | C |
| ATOM | 343 | OD1 | ASN | A | 58 | 34.140 | 31.983 | 10.018 | 1.00 | 41.34 | O |
| ATOM | 344 | ND2 | ASN | A | 58 | 34.241 | 33.617 | 11.639 | 1.00 | 41.14 | N |
| ATOM | 345 | N | GLU | A | 59 | 32.366 | 30.205 | 14.945 | 1.00 | 35.05 | N |
| ATOM | 346 | CA | GLU | A | 59 | 31.706 | 30.415 | 16.226 | 1.00 | 35.00 | C |
| ATOM | 347 | C | GLU | A | 59 | 30.481 | 31.314 | 16.133 | 1.00 | 33.86 | C |
| ATOM | 348 | O | GLU | A | 59 | 30.293 | 32.238 | 16.904 | 1.00 | 33.16 | O |
| ATOM | 349 | CB | GLU | A | 59 | 32.729 | 30.855 | 17.244 | 1.00 | 34.95 | C |
| ATOM | 350 | CG | GLU | A | 59 | 33.708 | 29.700 | 17.423 | 1.00 | 37.79 | C |
| ATOM | 351 | CD | GLU | A | 59 | 34.652 | 29.820 | 18.586 | 1.00 | 39.57 | C |
| ATOM | 352 | OE1 | GLU | A | 59 | 35.809 | 30.145 | 18.349 | 1.00 | 43.67 | O |
| ATOM | 353 | OE2 | GLU | A | 59 | 34.254 | 29.545 | 19.723 | 1.00 | 45.29 | O |
| ATOM | 354 | N | GLU | A | 60 | 29.644 | 30.995 | 15.157 | 1.00 | 32.92 | N |
| ATOM | 355 | CA | GLU | A | 60 | 28.359 | 31.641 | 14.983 | 1.00 | 32.66 | C |
| ATOM | 356 | C | GLU | A | 60 | 27.284 | 30.576 | 14.993 | 1.00 | 30.59 | C |
| ATOM | 357 | O | GLU | A | 60 | 27.456 | 29.485 | 14.461 | 1.00 | 30.47 | O |
| ATOM | 358 | CB | GLU | A | 60 | 28.312 | 32.400 | 13.685 | 1.00 | 33.20 | C |
| ATOM | 359 | CG | GLU | A | 60 | 29.384 | 33.454 | 13.615 | 1.00 | 38.62 | C |
| ATOM | 360 | CD | GLU | A | 60 | 28.955 | 34.617 | 12.762 | 1.00 | 45.73 | C |
| ATOM | 361 | OE1 | GLU | A | 60 | 29.075 | 34.553 | 11.519 | 1.00 | 48.47 | O |
| ATOM | 362 | OE2 | GLU | A | 60 | 28.466 | 35.587 | 13.367 | 1.00 | 53.89 | O |
| ATOM | 363 | N | PRO | A | 61 | 26.152 | 30.915 | 15.560 | 1.00 | 28.63 | N |
| ATOM | 364 | CA | PRO | A | 61 | 25.073 | 29.954 | 15.735 | 1.00 | 28.05 | C |
| ATOM | 365 | C | PRO | A | 61 | 24.462 | 29.451 | 14.443 | 1.00 | 27.61 | C |
| ATOM | 366 | O | PRO | A | 61 | 24.475 | 30.120 | 13.426 | 1.00 | 27.23 | O |
| ATOM | 367 | CB | PRO | A | 61 | 24.021 | 30.754 | 16.492 | 1.00 | 28.67 | C |
| ATOM | 368 | CG | PRO | A | 61 | 24.385 | 32.140 | 16.400 | 1.00 | 27.46 | C |
| ATOM | 369 | CD | PRO | A | 61 | 25.811 | 32.253 | 16.038 | 1.00 | 27.71 | C |
| ATOM | 370 | N | VAL | A | 62 | 23.936 | 28.237 | 14.475 | 1.00 | 27.43 | N |
| ATOM | 371 | CA | VAL | A | 62 | 23.254 | 27.685 | 13.317 | 1.00 | 27.09 | C |
| ATOM | 372 | C | VAL | A | 62 | 22.372 | 26.569 | 13.802 | 1.00 | 27.40 | C |
| ATOM | 373 | O | VAL | A | 62 | 22.707 | 25.893 | 14.780 | 1.00 | 27.79 | O |
| ATOM | 374 | CB | VAL | A | 62 | 24.219 | 27.181 | 12.270 | 1.00 | 27.04 | C |
| ATOM | 375 | CG1 | VAL | A | 62 | 25.106 | 26.166 | 12.829 | 1.00 | 27.34 | C |
| ATOM | 376 | CG2 | VAL | A | 62 | 23.473 | 26.659 | 11.037 | 1.00 | 27.58 | C |
| ATOM | 377 | N | VAL | A | 63 | 21.195 | 26.440 | 13.199 | 1.00 | 27.19 | N |
| ATOM | 378 | CA | VAL | A | 63 | 20.339 | 25.338 | 13.526 | 1.00 | 27.37 | C |
| ATOM | 379 | C | VAL | A | 63 | 20.540 | 24.324 | 12.383 | 1.00 | 27.33 | C |
| ATOM | 380 | O | VAL | A | 63 | 20.360 | 24.672 | 11.208 | 1.00 | 27.05 | O |
| ATOM | 381 | CB | VAL | A | 63 | 18.857 | 25.737 | 13.611 | 1.00 | 27.47 | C |
| ATOM | 382 | CG1 | VAL | A | 63 | 17.976 | 24.446 | 13.695 | 1.00 | 28.55 | C |
| ATOM | 383 | CG2 | VAL | A | 63 | 18.616 | 26.603 | 14.793 | 1.00 | 25.77 | C |
| ATOM | 384 | N | LEU | A | 64 | 20.933 | 23.114 | 12.743 | 1.00 | 27.26 | N |
| ATOM | 385 | CA | LEU | A | 64 | 21.119 | 22.001 | 11.820 | 1.00 | 28.51 | C |
| ATOM | 386 | C | LEU | A | 64 | 19.897 | 21.128 | 11.894 | 1.00 | 28.40 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 387 | O | LEU | A | 64 | 19.517 | 20.692 | 12.982 | 1.00 | 28.69 | O |
| ATOM | 388 | CB | LEU | A | 64 | 22.352 | 21.187 | 12.204 | 1.00 | 28.92 | C |
| ATOM | 389 | CG | LEU | A | 64 | 23.624 | 22.016 | 12.142 | 1.00 | 31.65 | C |
| ATOM | 390 | CD1 | LEU | A | 64 | 24.800 | 21.273 | 12.534 | 1.00 | 34.84 | C |
| ATOM | 391 | CD2 | LEU | A | 64 | 23.843 | 22.490 | 10.722 | 1.00 | 35.77 | C |
| ATOM | 392 | N | THR | A | 65 | 19.284 | 20.868 | 10.752 | 1.00 | 28.44 | N |
| ATOM | 393 | CA | THR | A | 65 | 18.003 | 20.164 | 10.721 | 1.00 | 29.54 | C |
| ATOM | 394 | C | THR | A | 65 | 18.054 | 18.659 | 10.534 | 1.00 | 29.40 | C |
| ATOM | 395 | O | THR | A | 65 | 17.046 | 17.985 | 10.799 | 1.00 | 29.20 | O |
| ATOM | 396 | CB | THR | A | 65 | 17.139 | 20.679 | 9.552 | 1.00 | 30.07 | C |
| ATOM | 397 | OG1 | THR | A | 65 | 17.879 | 20.569 | 8.318 | 1.00 | 30.75 | O |
| ATOM | 398 | CG2 | THR | A | 65 | 16.878 | 22.137 | 9.665 | 1.00 | 31.86 | C |
| ATOM | 399 | N | ASP | A | 66 | 19.183 | 18.150 | 10.059 | 1.00 | 29.30 | N |
| ATOM | 400 | CA | ASP | A | 66 | 19.323 | 16.722 | 9.719 | 1.00 | 29.78 | C |
| ATOM | 401 | C | ASP | A | 66 | 20.573 | 15.970 | 10.196 | 1.00 | 29.12 | C |
| ATOM | 402 | O | ASP | A | 66 | 21.081 | 15.141 | 9.432 | 1.00 | 29.09 | O |
| ATOM | 403 | CB | ASP | A | 66 | 19.301 | 16.582 | 8.195 | 1.00 | 29.41 | C |
| ATOM | 404 | CG | ASP | A | 66 | 20.274 | 17.507 | 7.525 | 1.00 | 32.36 | C |
| ATOM | 405 | OD1 | ASP | A | 66 | 20.924 | 18.319 | 8.230 | 1.00 | 34.87 | O |
| ATOM | 406 | OD2 | ASP | A | 66 | 20.447 | 17.534 | 6.287 | 1.00 | 35.70 | O |
| ATOM | 407 | N | THR | A | 67 | 21.078 | 16.254 | 11.404 | 1.00 | 28.05 | N |
| ATOM | 408 | CA | THR | A | 67 | 22.266 | 15.565 | 11.897 | 1.00 | 27.24 | C |
| ATOM | 409 | C | THR | A | 67 | 21.943 | 14.171 | 12.355 | 1.00 | 26.92 | C |
| ATOM | 410 | O | THR | A | 67 | 22.807 | 13.297 | 12.367 | 1.00 | 25.98 | O |
| ATOM | 411 | CB | THR | A | 67 | 22.856 | 16.258 | 13.134 | 1.00 | 27.78 | C |
| ATOM | 412 | OG1 | THR | A | 67 | 21.874 | 16.338 | 14.186 | 1.00 | 25.71 | O |
| ATOM | 413 | CG2 | THR | A | 67 | 23.268 | 17.664 | 12.820 | 1.00 | 29.22 | C |
| ATOM | 414 | N | ASN | A | 68 | 20.704 | 13.979 | 12.777 | 1.00 | 26.53 | N |
| ATOM | 415 | CA | ASN | A | 68 | 20.307 | 12.711 | 13.355 | 1.00 | 27.10 | C |
| ATOM | 416 | C | ASN | A | 68 | 21.075 | 12.499 | 14.647 | 1.00 | 26.46 | C |
| ATOM | 417 | O | ASN | A | 68 | 21.223 | 11.399 | 15.092 | 1.00 | 26.90 | O |
| ATOM | 418 | CB | ASN | A | 68 | 20.583 | 11.547 | 12.401 | 1.00 | 27.41 | C |
| ATOM | 419 | CG | ASN | A | 68 | 19.546 | 11.415 | 11.308 | 1.00 | 28.18 | C |
| ATOM | 420 | OD1 | ASN | A | 68 | 18.345 | 11.286 | 11.566 | 1.00 | 29.22 | O |
| ATOM | 421 | ND2 | ASN | A | 68 | 20.006 | 11.445 | 10.077 | 1.00 | 29.40 | N |
| ATOM | 422 | N | LEU | A | 69 | 21.585 | 13.569 | 15.227 | 1.00 | 26.58 | N |
| ATOM | 423 | CA | LEU | A | 69 | 22.429 | 13.481 | 16.427 | 1.00 | 26.67 | C |
| ATOM | 424 | C | LEU | A | 69 | 21.832 | 12.639 | 17.558 | 1.00 | 26.73 | C |
| ATOM | 425 | O | LEU | A | 69 | 22.550 | 11.822 | 18.166 | 1.00 | 27.74 | O |
| ATOM | 426 | CB | LEU | A | 69 | 22.739 | 14.870 | 16.968 | 1.00 | 26.04 | C |
| ATOM | 427 | CG | LEU | A | 69 | 23.677 | 14.904 | 18.157 | 1.00 | 26.23 | C |
| ATOM | 428 | CD1 | LEU | A | 69 | 24.986 | 14.168 | 17.894 | 1.00 | 27.92 | C |
| ATOM | 429 | CD2 | LEU | A | 69 | 23.976 | 16.343 | 18.556 | 1.00 | 24.74 | C |
| ATOM | 430 | N | VAL | A | 70 | 20.557 | 12.857 | 17.861 | 1.00 | 26.02 | N |
| ATOM | 431 | CA | VAL | A | 70 | 19.882 | 12.091 | 18.898 | 1.00 | 26.50 | C |
| ATOM | 432 | C | VAL | A | 70 | 18.673 | 11.364 | 18.345 | 1.00 | 26.71 | C |
| ATOM | 433 | O | VAL | A | 70 | 17.650 | 11.183 | 19.015 | 1.00 | 25.59 | O |
| ATOM | 434 | CB | VAL | A | 70 | 19.479 | 12.943 | 20.098 | 1.00 | 26.46 | C |
| ATOM | 435 | CG1 | VAL | A | 70 | 20.717 | 13.505 | 20.764 | 1.00 | 28.17 | C |
| ATOM | 436 | CG2 | VAL | A | 70 | 18.517 | 14.016 | 19.716 | 1.00 | 23.88 | C |
| ATOM | 437 | N | TYR | A | 71 | 18.832 | 10.920 | 17.113 | 1.00 | 27.86 | N |
| ATOM | 438 | CA | TYR | A | 71 | 17.791 | 10.159 | 16.451 | 1.00 | 29.60 | C |
| ATOM | 439 | C | TYR | A | 71 | 17.093 | 9.167 | 17.388 | 1.00 | 29.76 | C |
| ATOM | 440 | O | TYR | A | 71 | 15.905 | 9.202 | 17.478 | 1.00 | 30.54 | O |
| ATOM | 441 | CB | TYR | A | 71 | 18.326 | 9.459 | 15.208 | 1.00 | 29.31 | C |
| ATOM | 442 | CG | TYR | A | 71 | 17.347 | 8.479 | 14.686 | 1.00 | 31.42 | C |
| ATOM | 443 | CD1 | TYR | A | 71 | 16.136 | 8.884 | 14.120 | 1.00 | 31.39 | C |
| ATOM | 444 | CD2 | TYR | A | 71 | 17.610 | 7.107 | 14.779 | 1.00 | 32.30 | C |
| ATOM | 445 | CE1 | TYR | A | 71 | 15.223 | 7.905 | 13.641 | 1.00 | 31.86 | C |
| ATOM | 446 | CE2 | TYR | A | 71 | 16.736 | 6.181 | 14.317 | 1.00 | 29.75 | C |
| ATOM | 447 | CZ | TYR | A | 71 | 15.556 | 6.558 | 13.755 | 1.00 | 31.10 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 448 | OH | TYR A | 71 | 14.698 | 5.530 | 13.342 | 1.00 | 39.44 | O |
| ATOM | 449 | N | PRO A | 72 | 17.807 | 8.317 | 18.108 | 1.00 | 30.56 | N |
| ATOM | 450 | CA | PRO A | 72 | 17.150 | 7.336 | 18.991 | 1.00 | 30.85 | C |
| ATOM | 451 | C | PRO A | 72 | 16.389 | 7.914 | 20.158 | 1.00 | 30.85 | C |
| ATOM | 452 | O | PRO A | 72 | 15.549 | 7.233 | 20.750 | 1.00 | 30.12 | O |
| ATOM | 453 | CB | PRO A | 72 | 18.310 | 6.468 | 19.507 | 1.00 | 30.71 | C |
| ATOM | 454 | CG | PRO A | 72 | 19.420 | 6.692 | 18.515 | 1.00 | 31.79 | C |
| ATOM | 455 | CD | PRO A | 72 | 19.268 | 8.158 | 18.096 | 1.00 | 30.88 | C |
| ATOM | 456 | N | ALA A | 73 | 16.650 | 9.166 | 20.508 | 1.00 | 31.72 | N |
| ATOM | 457 | CA | ALA A | 73 | 15.918 | 9.743 | 21.627 | 1.00 | 31.71 | C |
| ATOM | 458 | C | ALA A | 73 | 14.596 | 10.371 | 21.172 | 1.00 | 31.83 | C |
| ATOM | 459 | O | ALA A | 73 | 13.786 | 10.808 | 22.000 | 1.00 | 31.52 | O |
| ATOM | 460 | CB | ALA A | 73 | 16.762 | 10.742 | 22.340 | 1.00 | 32.17 | C |
| ATOM | 461 | N | LEU A | 74 | 14.345 | 10.408 | 19.868 | 1.00 | 31.19 | N |
| ATOM | 462 | CA | LEU A | 74 | 13.108 | 11.028 | 19.439 | 1.00 | 32.01 | C |
| ATOM | 463 | C | LEU A | 74 | 11.856 | 10.343 | 19.965 | 1.00 | 32.30 | C |
| ATOM | 464 | O | LEU A | 74 | 10.807 | 10.914 | 19.963 | 1.00 | 31.90 | O |
| ATOM | 465 | CB | LEU A | 74 | 13.050 | 11.191 | 17.931 | 1.00 | 31.25 | C |
| ATOM | 466 | CG | LEU A | 74 | 14.140 | 12.103 | 17.400 | 1.00 | 34.53 | C |
| ATOM | 467 | CD1 | LEU A | 74 | 13.904 | 12.418 | 15.965 | 1.00 | 37.35 | C |
| ATOM | 468 | CD2 | LEU A | 74 | 14.264 | 13.436 | 18.200 | 1.00 | 34.44 | C |
| ATOM | 469 | N | LYS A | 75 | 11.963 | 9.100 | 20.396 | 1.00 | 34.18 | N |
| ATOM | 470 | CA | LYS A | 75 | 10.802 | 8.376 | 20.910 | 1.00 | 34.36 | C |
| ATOM | 471 | C | LYS A | 75 | 10.618 | 8.616 | 22.403 | 1.00 | 35.18 | C |
| ATOM | 472 | O | LYS A | 75 | 9.575 | 8.304 | 22.945 | 1.00 | 35.70 | O |
| ATOM | 473 | CB | LYS A | 75 | 10.950 | 6.876 | 20.631 | 1.00 | 34.51 | C |
| ATOM | 474 | CG | LYS A | 75 | 12.138 | 6.219 | 21.294 | 1.00 | 33.19 | C |
| ATOM | 475 | CD | LYS A | 75 | 12.302 | 4.754 | 20.834 | 1.00 | 31.54 | C |
| ATOM | 476 | CE | LYS A | 75 | 13.796 | 4.304 | 20.744 | 1.00 | 29.70 | C |
| ATOM | 477 | NZ | LYS A | 75 | 14.460 | 4.158 | 22.026 | 1.00 | 28.79 | N |
| ATOM | 478 | N | TRP A | 76 | 11.619 | 9.181 | 23.071 | 1.00 | 35.44 | N |
| ATOM | 479 | CA | TRP A | 76 | 11.517 | 9.426 | 24.495 | 1.00 | 36.05 | C |
| ATOM | 480 | C | TRP A | 76 | 10.307 | 10.264 | 24.893 | 1.00 | 37.47 | C |
| ATOM | 481 | O | TRP A | 76 | 9.958 | 11.222 | 24.212 | 1.00 | 38.43 | O |
| ATOM | 482 | CB | TRP A | 76 | 12.742 | 10.179 | 24.994 | 1.00 | 35.67 | C |
| ATOM | 483 | CG | TRP A | 76 | 13.980 | 9.395 | 24.963 | 1.00 | 33.87 | C |
| ATOM | 484 | CD1 | TRP A | 76 | 14.136 | 8.116 | 24.520 | 1.00 | 32.29 | C |
| ATOM | 485 | CD2 | TRP A | 76 | 15.252 | 9.821 | 25.409 | 1.00 | 30.36 | C |
| ATOM | 486 | NE1 | TRP A | 76 | 15.440 | 7.723 | 24.673 | 1.00 | 30.42 | N |
| ATOM | 487 | CE2 | TRP A | 76 | 16.143 | 8.754 | 25.221 | 1.00 | 28.82 | C |
| ATOM | 488 | CE3 | TRP A | 76 | 15.739 | 11.013 | 25.954 | 1.00 | 29.45 | C |
| ATOM | 489 | CZ2 | TRP A | 76 | 17.471 | 8.833 | 25.560 | 1.00 | 30.56 | C |
| ATOM | 490 | CZ3 | TRP A | 76 | 17.056 | 11.091 | 26.291 | 1.00 | 29.56 | C |
| ATOM | 491 | CH2 | TRP A | 76 | 17.917 | 10.017 | 26.092 | 1.00 | 30.20 | C |
| ATOM | 492 | N | ASP A | 77 | 9.698 | 9.894 | 26.014 | 1.00 | 38.14 | N |
| ATOM | 493 | CA | ASP A | 77 | 8.620 | 10.640 | 26.635 | 1.00 | 38.33 | C |
| ATOM | 494 | C | ASP A | 77 | 8.653 | 10.223 | 28.094 | 1.00 | 37.89 | C |
| ATOM | 495 | O | ASP A | 77 | 9.443 | 9.390 | 28.447 | 1.00 | 37.97 | O |
| ATOM | 496 | CB | ASP A | 77 | 7.283 | 10.353 | 25.974 | 1.00 | 38.71 | C |
| ATOM | 497 | CG | ASP A | 77 | 6.882 | 8.904 | 26.049 | 1.00 | 39.50 | C |
| ATOM | 498 | OD1 | ASP A | 77 | 7.414 | 8.107 | 26.867 | 1.00 | 41.50 | O |
| ATOM | 499 | OD2 | ASP A | 77 | 6.006 | 8.472 | 25.299 | 1.00 | 41.98 | O |
| ATOM | 500 | N | LEU A | 78 | 7.838 | 10.800 | 28.955 | 1.00 | 38.47 | N |
| ATOM | 501 | CA | LEU A | 78 | 7.941 | 10.481 | 30.375 | 1.00 | 39.09 | C |
| ATOM | 502 | C | LEU A | 78 | 7.734 | 9.002 | 30.662 | 1.00 | 39.89 | C |
| ATOM | 503 | O | LEU A | 78 | 8.421 | 8.423 | 31.507 | 1.00 | 40.19 | O |
| ATOM | 504 | CB | LEU A | 78 | 6.966 | 11.310 | 31.171 | 1.00 | 39.02 | C |
| ATOM | 505 | CG | LEU A | 78 | 7.169 | 12.815 | 31.042 | 1.00 | 41.51 | C |
| ATOM | 506 | CD1 | LEU A | 78 | 6.058 | 13.567 | 31.764 | 1.00 | 42.72 | C |
| ATOM | 507 | CD2 | LEU A | 78 | 8.522 | 13.216 | 31.618 | 1.00 | 42.31 | C |
| ATOM | 508 | N | GLU A | 79 | 6.795 | 8.369 | 29.971 | 1.00 | 40.66 | N |

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ATOM    509  CA  GLU A  79       6.557   6.948  30.212  1.00 41.43           C
ATOM    510  C   GLU A  79       7.794   6.086  29.909  1.00 40.84           C
ATOM    511  O   GLU A  79       8.228   5.283  30.742  1.00 40.45           O
ATOM    512  CB  GLU A  79       5.343   6.458  29.418  1.00 42.10           C
ATOM    513  CG  GLU A  79       5.023   4.998  29.658  1.00 45.06           C
ATOM    514  CD  GLU A  79       3.840   4.525  28.846  1.00 49.74           C
ATOM    515  OE1 GLU A  79       3.436   5.254  27.914  1.00 52.37           O
ATOM    516  OE2 GLU A  79       3.316   3.426  29.150  1.00 53.21           O
ATOM    517  N   TYR A  80       8.361   6.248  28.718  1.00 40.43           N
ATOM    518  CA  TYR A  80       9.559   5.495  28.362  1.00 40.14           C
ATOM    519  C   TYR A  80      10.750   5.765  29.297  1.00 40.06           C
ATOM    520  O   TYR A  80      11.485   4.844  29.664  1.00 39.72           O
ATOM    521  CB  TYR A  80       9.946   5.832  26.946  1.00 39.96           C
ATOM    522  CG  TYR A  80      11.193   5.147  26.420  1.00 39.51           C
ATOM    523  CD1 TYR A  80      11.118   3.897  25.804  1.00 38.93           C
ATOM    524  CD2 TYR A  80      12.433   5.768  26.490  1.00 36.89           C
ATOM    525  CE1 TYR A  80      12.253   3.277  25.290  1.00 38.08           C
ATOM    526  CE2 TYR A  80      13.562   5.154  25.993  1.00 38.15           C
ATOM    527  CZ  TYR A  80      13.468   3.915  25.379  1.00 39.06           C
ATOM    528  OH  TYR A  80      14.604   3.319  24.863  1.00 38.99           O
ATOM    529  N   LEU A  81      10.935   7.017  29.688  1.00 39.68           N
ATOM    530  CA  LEU A  81      12.061   7.362  30.565  1.00 40.01           C
ATOM    531  C   LEU A  81      11.858   6.806  31.978  1.00 39.86           C
ATOM    532  O   LEU A  81      12.792   6.284  32.608  1.00 39.47           O
ATOM    533  CB  LEU A  81      12.314   8.889  30.604  1.00 39.50           C
ATOM    534  CG  LEU A  81      12.765   9.532  29.287  1.00 39.76           C
ATOM    535  CD1 LEU A  81      12.805  11.045  29.402  1.00 39.84           C
ATOM    536  CD2 LEU A  81      14.117   9.018  28.840  1.00 39.32           C
ATOM    537  N   GLN A  82      10.645   6.932  32.482  1.00 40.38           N
ATOM    538  CA  GLN A  82      10.346   6.415  33.804  1.00 41.02           C
ATOM    539  C   GLN A  82      10.612   4.920  33.799  1.00 40.84           C
ATOM    540  O   GLN A  82      11.193   4.379  34.711  1.00 40.35           O
ATOM    541  CB  GLN A  82       8.900   6.688  34.164  1.00 41.40           C
ATOM    542  CG  GLN A  82       8.447   5.906  35.351  1.00 42.97           C
ATOM    543  CD  GLN A  82       7.291   6.560  36.099  1.00 45.14           C
ATOM    544  OE1 GLN A  82       6.662   7.502  35.616  1.00 44.10           O
ATOM    545  NE2 GLN A  82       7.003   6.039  37.287  1.00 48.04           N
ATOM    546  N   GLU A  83      10.222   4.256  32.728  1.00 41.35           N
ATOM    547  CA  GLU A  83      10.442   2.816  32.620  1.00 41.46           C
ATOM    548  C   GLU A  83      11.926   2.444  32.465  1.00 40.81           C
ATOM    549  O   GLU A  83      12.350   1.407  32.958  1.00 41.13           O
ATOM    550  CB  GLU A  83       9.610   2.243  31.472  1.00 41.27           C
ATOM    551  CG  GLU A  83       9.609   0.728  31.366  1.00 44.77           C
ATOM    552  CD  GLU A  83       8.878   0.018  32.514  1.00 49.16           C
ATOM    553  OE1 GLU A  83       8.219   0.672  33.347  1.00 52.26           O
ATOM    554  OE2 GLU A  83       8.978  -1.220  32.606  1.00 53.23           O
ATOM    555  N   ASN A  84      12.743   3.298  31.854  1.00 39.81           N
ATOM    556  CA  ASN A  84      14.099   2.859  31.515  1.00 38.82           C
ATOM    557  C   ASN A  84      15.290   3.611  32.048  1.00 38.20           C
ATOM    558  O   ASN A  84      16.402   3.117  31.919  1.00 36.98           O
ATOM    559  CB  ASN A  84      14.244   2.828  29.995  1.00 38.83           C
ATOM    560  CG  ASN A  84      13.301   1.865  29.349  1.00 38.45           C
ATOM    561  OD1 ASN A  84      13.307   0.670  29.664  1.00 40.40           O
ATOM    562  ND2 ASN A  84      12.480   2.365  28.441  1.00 35.77           N
ATOM    563  N   ILE A  85      15.088   4.781  32.645  1.00 38.08           N
ATOM    564  CA  ILE A  85      16.226   5.598  32.998  1.00 38.57           C
ATOM    565  C   ILE A  85      16.929   5.280  34.307  1.00 38.70           C
ATOM    566  O   ILE A  85      17.849   5.993  34.702  1.00 39.78           O
ATOM    567  CB  ILE A  85      15.827   7.056  32.932  1.00 39.02           C
ATOM    568  CG1 ILE A  85      17.001   7.891  32.418  1.00 39.43           C
ATOM    569  CG2 ILE A  85      15.291   7.544  34.266  1.00 39.22           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 570 | CD1 | ILE | A | 85 | 16.618 | 9.347 | 32.148 | 1.00 | 40.41 | C |
| ATOM | 571 | N | GLY | A | 86 | 16.513 | 4.227 | 34.993 | 1.00 | 38.59 | N |
| ATOM | 572 | CA | GLY | A | 86 | 17.208 | 3.801 | 36.199 | 1.00 | 38.15 | C |
| ATOM | 573 | C | GLY | A | 86 | 16.658 | 4.386 | 37.476 | 1.00 | 37.92 | C |
| ATOM | 574 | O | GLY | A | 86 | 15.652 | 5.097 | 37.461 | 1.00 | 37.90 | O |
| ATOM | 575 | N | ASN | A | 87 | 17.359 | 4.113 | 38.574 | 1.00 | 37.70 | N |
| ATOM | 576 | CA | ASN | A | 87 | 16.941 | 4.542 | 39.899 | 1.00 | 37.34 | C |
| ATOM | 577 | C | ASN | A | 87 | 17.898 | 5.576 | 40.487 | 1.00 | 36.99 | C |
| ATOM | 578 | O | ASN | A | 87 | 17.920 | 5.807 | 41.710 | 1.00 | 36.36 | O |
| ATOM | 579 | CB | ASN | A | 87 | 16.786 | 3.306 | 40.840 | 1.00 | 37.40 | C |
| ATOM | 580 | N | GLY | A | 88 | 18.676 | 6.224 | 39.618 | 1.00 | 37.00 | N |
| ATOM | 581 | CA | GLY | A | 88 | 19.593 | 7.272 | 40.056 | 1.00 | 36.90 | C |
| ATOM | 582 | C | GLY | A | 88 | 18.855 | 8.506 | 40.541 | 1.00 | 36.61 | C |
| ATOM | 583 | O | GLY | A | 88 | 17.673 | 8.648 | 40.298 | 1.00 | 36.55 | O |
| ATOM | 584 | N | ASP | A | 89 | 19.532 | 9.392 | 41.250 | 1.00 | 37.05 | N |
| ATOM | 585 | CA | ASP | A | 89 | 18.882 | 10.640 | 41.687 | 1.00 | 37.92 | C |
| ATOM | 586 | C | ASP | A | 89 | 18.812 | 11.654 | 40.548 | 1.00 | 37.52 | C |
| ATOM | 587 | O | ASP | A | 89 | 19.724 | 11.713 | 39.730 | 1.00 | 37.73 | O |
| ATOM | 588 | CB | ASP | A | 89 | 19.639 | 11.281 | 42.840 | 1.00 | 38.02 | C |
| ATOM | 589 | CG | ASP | A | 89 | 19.342 | 10.639 | 44.165 | 1.00 | 40.19 | C |
| ATOM | 590 | OD1 | ASP | A | 89 | 18.398 | 9.813 | 44.252 | 1.00 | 44.15 | O |
| ATOM | 591 | OD2 | ASP | A | 89 | 20.002 | 10.918 | 45.186 | 1.00 | 42.25 | O |
| ATOM | 592 | N | PHE | A | 90 | 17.734 | 12.438 | 40.491 | 1.00 | 37.19 | N |
| ATOM | 593 | CA | PHE | A | 90 | 17.638 | 13.546 | 39.520 | 1.00 | 36.65 | C |
| ATOM | 594 | C | PHE | A | 90 | 17.435 | 14.912 | 40.182 | 1.00 | 36.57 | C |
| ATOM | 595 | O | PHE | A | 90 | 16.551 | 15.078 | 41.015 | 1.00 | 36.80 | O |
| ATOM | 596 | CB | PHE | A | 90 | 16.512 | 13.310 | 38.516 | 1.00 | 35.79 | C |
| ATOM | 597 | CG | PHE | A | 90 | 16.793 | 12.200 | 37.551 | 1.00 | 35.34 | C |
| ATOM | 598 | CD1 | PHE | A | 90 | 16.627 | 10.870 | 37.931 | 1.00 | 34.10 | C |
| ATOM | 599 | CD2 | PHE | A | 90 | 17.235 | 12.472 | 36.275 | 1.00 | 34.19 | C |
| ATOM | 600 | CE1 | PHE | A | 90 | 16.875 | 9.854 | 37.061 | 1.00 | 31.47 | C |
| ATOM | 601 | CE2 | PHE | A | 90 | 17.488 | 11.452 | 35.404 | 1.00 | 35.32 | C |
| ATOM | 602 | CZ | PHE | A | 90 | 17.315 | 10.123 | 35.813 | 1.00 | 34.26 | C |
| ATOM | 603 | N | SER | A | 91 | 18.257 | 15.886 | 39.803 | 1.00 | 36.85 | N |
| ATOM | 604 | CA | SER | A | 91 | 18.077 | 17.264 | 40.278 | 1.00 | 37.16 | C |
| ATOM | 605 | C | SER | A | 91 | 16.856 | 17.884 | 39.612 | 1.00 | 37.28 | C |
| ATOM | 606 | O | SER | A | 91 | 16.761 | 17.912 | 38.392 | 1.00 | 36.72 | O |
| ATOM | 607 | CB | SER | A | 91 | 19.278 | 18.146 | 39.971 | 1.00 | 36.75 | C |
| ATOM | 608 | OG | SER | A | 91 | 20.470 | 17.600 | 40.456 | 1.00 | 35.79 | O |
| ATOM | 609 | N | VAL | A | 92 | 15.938 | 18.374 | 40.434 | 1.00 | 37.83 | N |
| ATOM | 610 | CA | VAL | A | 92 | 14.740 | 19.022 | 39.963 | 1.00 | 38.40 | C |
| ATOM | 611 | C | VAL | A | 92 | 14.549 | 20.334 | 40.690 | 1.00 | 39.41 | C |
| ATOM | 612 | O | VAL | A | 92 | 14.465 | 20.394 | 41.941 | 1.00 | 39.08 | O |
| ATOM | 613 | CB | VAL | A | 92 | 13.507 | 18.227 | 40.298 | 1.00 | 38.96 | C |
| ATOM | 614 | CG1 | VAL | A | 92 | 12.270 | 19.005 | 39.893 | 1.00 | 38.57 | C |
| ATOM | 615 | CG2 | VAL | A | 92 | 13.556 | 16.837 | 39.651 | 1.00 | 39.45 | C |
| ATOM | 616 | N | TYR | A | 93 | 14.426 | 21.386 | 39.895 | 1.00 | 39.95 | N |
| ATOM | 617 | CA | TYR | A | 93 | 14.214 | 22.701 | 40.419 | 1.00 | 40.34 | C |
| ATOM | 618 | C | TYR | A | 93 | 12.756 | 22.950 | 40.459 | 1.00 | 40.76 | C |
| ATOM | 619 | O | TYR | A | 93 | 11.999 | 22.493 | 39.583 | 1.00 | 40.39 | O |
| ATOM | 620 | CB | TYR | A | 93 | 14.897 | 23.729 | 39.529 | 1.00 | 40.89 | C |
| ATOM | 621 | CG | TYR | A | 93 | 16.369 | 23.580 | 39.627 | 1.00 | 40.80 | C |
| ATOM | 622 | CD1 | TYR | A | 93 | 17.067 | 24.135 | 40.681 | 1.00 | 40.79 | C |
| ATOM | 623 | CD2 | TYR | A | 93 | 17.042 | 22.801 | 38.743 | 1.00 | 41.05 | C |
| ATOM | 624 | CE1 | TYR | A | 93 | 18.395 | 23.953 | 40.802 | 1.00 | 41.05 | C |
| ATOM | 625 | CE2 | TYR | A | 93 | 18.363 | 22.629 | 38.852 | 1.00 | 42.75 | C |
| ATOM | 626 | CZ | TYR | A | 93 | 19.037 | 23.204 | 39.881 | 1.00 | 42.45 | C |
| ATOM | 627 | OH | TYR | A | 93 | 20.372 | 22.965 | 39.971 | 1.00 | 47.63 | O |
| ATOM | 628 | N | SER | A | 94 | 12.385 | 23.699 | 41.482 | 1.00 | 41.70 | N |
| ATOM | 629 | CA | SER | A | 94 | 11.014 | 24.053 | 41.743 | 1.00 | 42.70 | C |
| ATOM | 630 | C | SER | A | 94 | 10.965 | 25.565 | 41.855 | 1.00 | 43.09 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 631 | O | SER | A | 94 | 11.851 | 26.181 | 42.441 | 1.00 | 43.63 | O |
| ATOM | 632 | CB | SER | A | 94 | 10.570 | 23.415 | 43.051 | 1.00 | 42.76 | C |
| ATOM | 633 | OG | SER | A | 94 | 9.258 | 23.841 | 43.395 | 1.00 | 45.05 | O |
| ATOM | 634 | N | ALA | A | 95 | 9.929 | 26.171 | 41.308 | 1.00 | 43.42 | N |
| ATOM | 635 | CA | ALA | A | 95 | 9.839 | 27.607 | 41.323 | 1.00 | 43.49 | C |
| ATOM | 636 | C | ALA | A | 95 | 8.416 | 28.083 | 41.281 | 1.00 | 43.87 | C |
| ATOM | 637 | O | ALA | A | 95 | 7.520 | 27.416 | 40.789 | 1.00 | 43.95 | O |
| ATOM | 638 | CB | ALA | A | 95 | 10.572 | 28.164 | 40.145 | 1.00 | 43.70 | C |
| ATOM | 639 | N | SER | A | 96 | 8.219 | 29.287 | 41.770 | 1.00 | 44.66 | N |
| ATOM | 640 | CA | SER | A | 96 | 6.901 | 29.866 | 41.757 | 1.00 | 45.08 | C |
| ATOM | 641 | C | SER | A | 96 | 6.767 | 30.914 | 40.668 | 1.00 | 44.27 | C |
| ATOM | 642 | O | SER | A | 96 | 5.783 | 31.636 | 40.637 | 1.00 | 45.20 | O |
| ATOM | 643 | CB | SER | A | 96 | 6.604 | 30.510 | 43.095 | 1.00 | 45.33 | C |
| ATOM | 644 | OG | SER | A | 96 | 5.384 | 31.199 | 42.973 | 1.00 | 47.96 | O |
| ATOM | 645 | N | THR | A | 97 | 7.776 | 31.034 | 39.819 | 1.00 | 42.95 | N |
| ATOM | 646 | CA | THR | A | 97 | 7.738 | 31.962 | 38.688 | 1.00 | 42.08 | C |
| ATOM | 647 | C | THR | A | 97 | 8.103 | 31.184 | 37.461 | 1.00 | 40.94 | C |
| ATOM | 648 | O | THR | A | 97 | 8.604 | 30.095 | 37.584 | 1.00 | 40.73 | O |
| ATOM | 649 | CB | THR | A | 97 | 8.779 | 33.088 | 38.826 | 1.00 | 42.48 | C |
| ATOM | 650 | OG1 | THR | A | 97 | 8.964 | 33.707 | 37.546 | 1.00 | 43.60 | O |
| ATOM | 651 | CG2 | THR | A | 97 | 10.209 | 32.544 | 39.156 | 1.00 | 42.12 | C |
| ATOM | 652 | N | HIS | A | 98 | 7.904 | 31.734 | 36.275 | 1.00 | 40.18 | N |
| ATOM | 653 | CA | HIS | A | 98 | 8.319 | 31.012 | 35.074 | 1.00 | 40.09 | C |
| ATOM | 654 | C | HIS | A | 98 | 9.840 | 31.036 | 34.883 | 1.00 | 39.78 | C |
| ATOM | 655 | O | HIS | A | 98 | 10.376 | 30.277 | 34.078 | 1.00 | 38.48 | O |
| ATOM | 656 | CB | HIS | A | 98 | 7.660 | 31.580 | 33.824 | 1.00 | 40.00 | C |
| ATOM | 657 | CG | HIS | A | 98 | 7.947 | 33.028 | 33.582 | 1.00 | 40.56 | C |
| ATOM | 658 | ND1 | HIS | A | 98 | 7.297 | 34.041 | 34.259 | 1.00 | 40.13 | N |
| ATOM | 659 | CD2 | HIS | A | 98 | 8.805 | 33.640 | 32.729 | 1.00 | 42.26 | C |
| ATOM | 660 | CE1 | HIS | A | 98 | 7.741 | 35.212 | 33.841 | 1.00 | 37.08 | C |
| ATOM | 661 | NE2 | HIS | A | 98 | 8.661 | 35.002 | 32.915 | 1.00 | 39.74 | N |
| ATOM | 662 | N | LYS | A | 99 | 10.526 | 31.883 | 35.652 | 1.00 | 39.73 | N |
| ATOM | 663 | CA | LYS | A | 99 | 11.948 | 32.082 | 35.476 | 1.00 | 40.45 | C |
| ATOM | 664 | C | LYS | A | 99 | 12.861 | 31.221 | 36.332 | 1.00 | 40.34 | C |
| ATOM | 665 | O | LYS | A | 99 | 12.904 | 31.376 | 37.554 | 1.00 | 41.93 | O |
| ATOM | 666 | CB | LYS | A | 99 | 12.279 | 33.535 | 35.730 | 1.00 | 40.89 | C |
| ATOM | 667 | CG | LYS | A | 99 | 11.819 | 34.443 | 34.624 | 1.00 | 43.12 | C |
| ATOM | 668 | CD | LYS | A | 99 | 12.466 | 35.806 | 34.753 | 1.00 | 46.04 | C |
| ATOM | 669 | CE | LYS | A | 99 | 11.733 | 36.727 | 35.711 | 1.00 | 48.26 | C |
| ATOM | 670 | NZ | LYS | A | 99 | 10.662 | 37.495 | 35.003 | 1.00 | 49.55 | N |
| ATOM | 671 | N | PHE | A | 100 | 13.622 | 30.335 | 35.700 | 1.00 | 39.70 | N |
| ATOM | 672 | CA | PHE | A | 100 | 14.554 | 29.487 | 36.447 | 1.00 | 39.48 | C |
| ATOM | 673 | C | PHE | A | 100 | 16.001 | 30.011 | 36.390 | 1.00 | 39.52 | C |
| ATOM | 674 | O | PHE | A | 100 | 16.874 | 29.435 | 35.718 | 1.00 | 38.87 | O |
| ATOM | 675 | CB | PHE | A | 100 | 14.485 | 28.056 | 35.939 | 1.00 | 39.33 | C |
| ATOM | 676 | CG | PHE | A | 100 | 13.266 | 27.328 | 36.377 | 1.00 | 38.47 | C |
| ATOM | 677 | CD1 | PHE | A | 100 | 12.059 | 27.519 | 35.725 | 1.00 | 36.20 | C |
| ATOM | 678 | CD2 | PHE | A | 100 | 13.327 | 26.441 | 37.443 | 1.00 | 37.31 | C |
| ATOM | 679 | CE1 | PHE | A | 100 | 10.960 | 26.846 | 36.125 | 1.00 | 36.52 | C |
| ATOM | 680 | CE2 | PHE | A | 100 | 12.212 | 25.751 | 37.849 | 1.00 | 36.40 | C |
| ATOM | 681 | CZ | PHE | A | 100 | 11.037 | 25.946 | 37.206 | 1.00 | 36.52 | C |
| ATOM | 682 | N | LEU | A | 101 | 16.244 | 31.130 | 37.066 | 1.00 | 39.53 | N |
| ATOM | 683 | CA | LEU | A | 101 | 17.592 | 31.667 | 37.170 | 1.00 | 39.36 | C |
| ATOM | 684 | C | LEU | A | 101 | 18.548 | 30.642 | 37.787 | 1.00 | 39.88 | C |
| ATOM | 685 | O | LEU | A | 101 | 18.345 | 30.152 | 38.899 | 1.00 | 39.47 | O |
| ATOM | 686 | CB | LEU | A | 101 | 17.574 | 32.912 | 38.036 | 1.00 | 39.37 | C |
| ATOM | 687 | CG | LEU | A | 101 | 18.828 | 33.777 | 38.071 | 1.00 | 39.44 | C |
| ATOM | 688 | CD1 | LEU | A | 101 | 19.258 | 34.290 | 36.693 | 1.00 | 37.56 | C |
| ATOM | 689 | CD2 | LEU | A | 101 | 18.546 | 34.926 | 39.008 | 1.00 | 39.90 | C |
| ATOM | 690 | N | TYR | A | 102 | 19.578 | 30.297 | 37.032 | 1.00 | 41.10 | N |
| ATOM | 691 | CA | TYR | A | 102 | 20.623 | 29.415 | 37.507 | 1.00 | 41.59 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 692 | C | TYR A 102 | 21.439 | 30.097 | 38.611 | 1.00 | 42.23 | | C |
| ATOM | 693 | O | TYR A 102 | 21.778 | 31.296 | 38.500 | 1.00 | 42.28 | | O |
| ATOM | 694 | CB | TYR A 102 | 21.580 | 29.048 | 36.370 | 1.00 | 41.49 | | C |
| ATOM | 695 | CG | TYR A 102 | 22.706 | 28.209 | 36.894 | 1.00 | 43.02 | | C |
| ATOM | 696 | CD1 | TYR A 102 | 22.507 | 26.864 | 37.200 | 1.00 | 42.85 | | C |
| ATOM | 697 | CD2 | TYR A 102 | 23.941 | 28.761 | 37.150 | 1.00 | 43.85 | | C |
| ATOM | 698 | CE1 | TYR A 102 | 23.504 | 26.110 | 37.725 | 1.00 | 45.04 | | C |
| ATOM | 699 | CE2 | TYR A 102 | 24.942 | 28.005 | 37.696 | 1.00 | 46.05 | | C |
| ATOM | 700 | CZ | TYR A 102 | 24.725 | 26.681 | 37.984 | 1.00 | 46.73 | | C |
| ATOM | 701 | OH | TYR A 102 | 25.752 | 25.915 | 38.544 | 1.00 | 52.49 | | O |
| ATOM | 702 | N | TYR A 103 | 21.759 | 29.340 | 39.657 | 1.00 | 42.12 | | N |
| ATOM | 703 | CA | TYR A 103 | 22.665 | 29.832 | 40.690 | 1.00 | 42.58 | | C |
| ATOM | 704 | C | TYR A 103 | 23.632 | 28.750 | 41.207 | 1.00 | 41.98 | | C |
| ATOM | 705 | O | TYR A 103 | 23.333 | 27.560 | 41.237 | 1.00 | 42.05 | | O |
| ATOM | 706 | CB | TYR A 103 | 21.901 | 30.435 | 41.843 | 1.00 | 43.03 | | C |
| ATOM | 707 | CG | TYR A 103 | 20.964 | 29.493 | 42.477 | 1.00 | 44.79 | | C |
| ATOM | 708 | CD1 | TYR A 103 | 19.691 | 29.333 | 41.971 | 1.00 | 47.69 | | C |
| ATOM | 709 | CD2 | TYR A 103 | 21.338 | 28.769 | 43.590 | 1.00 | 49.51 | | C |
| ATOM | 710 | CE1 | TYR A 103 | 18.798 | 28.456 | 42.544 | 1.00 | 50.63 | | C |
| ATOM | 711 | CE2 | TYR A 103 | 20.449 | 27.890 | 44.202 | 1.00 | 52.43 | | C |
| ATOM | 712 | CZ | TYR A 103 | 19.181 | 27.736 | 43.658 | 1.00 | 52.68 | | C |
| ATOM | 713 | OH | TYR A 103 | 18.297 | 26.875 | 44.234 | 1.00 | 56.40 | | O |
| ATOM | 714 | N | ASP A 104 | 24.809 | 29.190 | 41.603 | 1.00 | 41.00 | | N |
| ATOM | 715 | CA | ASP A 104 | 25.844 | 28.288 | 42.026 | 1.00 | 40.33 | | C |
| ATOM | 716 | C | ASP A 104 | 25.842 | 28.250 | 43.530 | 1.00 | 39.98 | | C |
| ATOM | 717 | O | ASP A 104 | 26.177 | 29.224 | 44.219 | 1.00 | 38.58 | | O |
| ATOM | 718 | CB | ASP A 104 | 27.169 | 28.768 | 41.492 | 1.00 | 40.13 | | C |
| ATOM | 719 | CG | ASP A 104 | 28.310 | 27.929 | 41.958 | 1.00 | 42.26 | | C |
| ATOM | 720 | OD1 | ASP A 104 | 28.117 | 27.151 | 42.942 | 1.00 | 44.33 | | O |
| ATOM | 721 | OD2 | ASP A 104 | 29.429 | 27.989 | 41.393 | 1.00 | 42.30 | | O |
| ATOM | 722 | N | GLU A 105 | 25.425 | 27.110 | 44.041 | 1.00 | 40.20 | | N |
| ATOM | 723 | CA | GLU A 105 | 25.294 | 26.950 | 45.472 | 1.00 | 40.26 | | C |
| ATOM | 724 | C | GLU A 105 | 26.605 | 27.213 | 46.228 | 1.00 | 39.92 | | C |
| ATOM | 725 | O | GLU A 105 | 26.577 | 27.824 | 47.293 | 1.00 | 40.11 | | O |
| ATOM | 726 | CB | GLU A 105 | 24.747 | 25.570 | 45.744 | 1.00 | 40.54 | | C |
| ATOM | 727 | CG | GLU A 105 | 23.245 | 25.502 | 45.533 | 1.00 | 42.55 | | C |
| ATOM | 728 | CD | GLU A 105 | 22.709 | 24.086 | 45.506 | 1.00 | 44.11 | | C |
| ATOM | 729 | OE1 | GLU A 105 | 23.178 | 23.251 | 46.323 | 1.00 | 46.78 | | O |
| ATOM | 730 | OE2 | GLU A 105 | 21.801 | 23.815 | 44.684 | 1.00 | 42.74 | | O |
| ATOM | 731 | N | LYS A 106 | 27.748 | 26.819 | 45.661 | 1.00 | 39.52 | | N |
| ATOM | 732 | CA | LYS A 106 | 29.041 | 26.991 | 46.336 | 1.00 | 39.53 | | C |
| ATOM | 733 | C | LYS A 106 | 29.370 | 28.419 | 46.623 | 1.00 | 39.68 | | C |
| ATOM | 734 | O | LYS A 106 | 30.199 | 28.697 | 47.471 | 1.00 | 40.24 | | O |
| ATOM | 735 | CB | LYS A 106 | 30.221 | 26.479 | 45.504 | 1.00 | 39.89 | | C |
| ATOM | 736 | CG | LYS A 106 | 30.257 | 24.976 | 45.143 | 1.00 | 40.25 | | C |
| ATOM | 737 | N | LYS A 107 | 28.747 | 29.333 | 45.894 | 1.00 | 40.07 | | N |
| ATOM | 738 | CA | LYS A 107 | 29.043 | 30.740 | 46.031 | 1.00 | 39.35 | | C |
| ATOM | 739 | C | LYS A 107 | 28.061 | 31.421 | 46.937 | 1.00 | 39.82 | | C |
| ATOM | 740 | O | LYS A 107 | 28.208 | 32.586 | 47.188 | 1.00 | 39.28 | | O |
| ATOM | 741 | CB | LYS A 107 | 29.050 | 31.410 | 44.645 | 1.00 | 39.29 | | C |
| ATOM | 742 | CG | LYS A 107 | 30.329 | 31.155 | 43.827 | 1.00 | 37.47 | | C |
| ATOM | 743 | CD | LYS A 107 | 30.286 | 31.702 | 42.406 | 1.00 | 34.55 | | C |
| ATOM | 744 | CE | LYS A 107 | 31.606 | 31.470 | 41.651 | 1.00 | 33.57 | | C |
| ATOM | 745 | NZ | LYS A 107 | 31.607 | 31.880 | 40.178 | 1.00 | 30.95 | | N |
| ATOM | 746 | N | MET A 108 | 27.071 | 30.707 | 47.458 | 1.00 | 41.78 | | N |
| ATOM | 747 | CA | MET A 108 | 26.079 | 31.341 | 48.341 | 1.00 | 43.69 | | C |
| ATOM | 748 | C | MET A 108 | 26.621 | 31.950 | 49.646 | 1.00 | 44.68 | | C |
| ATOM | 749 | O | MET A 108 | 26.154 | 33.004 | 50.061 | 1.00 | 44.99 | | O |
| ATOM | 750 | CB | MET A 108 | 24.923 | 30.396 | 48.594 | 1.00 | 44.05 | | C |
| ATOM | 751 | CG | MET A 108 | 24.195 | 30.105 | 47.282 | 1.00 | 46.49 | | C |
| ATOM | 752 | SD | MET A 108 | 22.723 | 29.125 | 47.315 | 1.00 | 51.54 | | S |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 753 | CE | MET | A | 108 | 21.653 | 30.080 | 48.484 | 1.00 | 51.43 | C |
| ATOM | 754 | N | ALA | A | 109 | 27.630 | 31.341 | 50.254 | 1.00 | 46.34 | N |
| ATOM | 755 | CA | ALA | A | 109 | 28.211 | 31.855 | 51.510 | 1.00 | 47.87 | C |
| ATOM | 756 | C | ALA | A | 109 | 28.697 | 33.308 | 51.406 | 1.00 | 49.27 | C |
| ATOM | 757 | O | ALA | A | 109 | 28.533 | 34.114 | 52.323 | 1.00 | 49.44 | O |
| ATOM | 758 | CB | ALA | A | 109 | 29.355 | 30.958 | 51.960 | 1.00 | 47.63 | C |
| ATOM | 759 | N | ASN | A | 110 | 29.276 | 33.651 | 50.269 | 1.00 | 50.88 | N |
| ATOM | 760 | CA | ASN | A | 110 | 29.792 | 35.004 | 50.069 | 1.00 | 51.99 | C |
| ATOM | 761 | C | ASN | A | 110 | 28.732 | 36.070 | 49.736 | 1.00 | 51.88 | C |
| ATOM | 762 | O | ASN | A | 110 | 29.038 | 37.252 | 49.562 | 1.00 | 51.14 | O |
| ATOM | 763 | CB | ASN | A | 110 | 30.876 | 34.939 | 48.994 | 1.00 | 52.43 | C |
| ATOM | 764 | CG | ASN | A | 110 | 32.077 | 34.080 | 49.433 | 1.00 | 54.41 | C |
| ATOM | 765 | OD1 | ASN | A | 110 | 32.460 | 34.050 | 50.624 | 1.00 | 54.72 | O |
| ATOM | 766 | ND2 | ASN | A | 110 | 32.663 | 33.373 | 48.478 | 1.00 | 56.75 | N |
| ATOM | 767 | N | PHE | A | 111 | 27.484 | 35.651 | 49.632 | 1.00 | 52.59 | N |
| ATOM | 768 | CA | PHE | A | 111 | 26.404 | 36.598 | 49.409 | 1.00 | 53.32 | C |
| ATOM | 769 | C | PHE | A | 111 | 25.202 | 36.180 | 50.261 | 1.00 | 54.75 | C |
| ATOM | 770 | O | PHE | A | 111 | 24.149 | 35.801 | 49.749 | 1.00 | 54.37 | O |
| ATOM | 771 | CB | PHE | A | 111 | 26.053 | 36.693 | 47.923 | 1.00 | 52.83 | C |
| ATOM | 772 | CG | PHE | A | 111 | 27.058 | 37.461 | 47.107 | 1.00 | 50.42 | C |
| ATOM | 773 | CD1 | PHE | A | 111 | 28.283 | 36.907 | 46.791 | 1.00 | 49.93 | C |
| ATOM | 774 | CD2 | PHE | A | 111 | 26.781 | 38.729 | 46.658 | 1.00 | 48.60 | C |
| ATOM | 775 | CE1 | PHE | A | 111 | 29.205 | 37.609 | 46.044 | 1.00 | 49.18 | C |
| ATOM | 776 | CE2 | PHE | A | 111 | 27.701 | 39.429 | 45.904 | 1.00 | 47.91 | C |
| ATOM | 777 | CZ | PHE | A | 111 | 28.910 | 38.869 | 45.601 | 1.00 | 47.42 | C |
| ATOM | 778 | N | GLN | A | 112 | 25.376 | 36.279 | 51.576 | 1.00 | 56.74 | N |
| ATOM | 779 | CA | GLN | A | 112 | 24.353 | 35.855 | 52.536 | 1.00 | 58.14 | C |
| ATOM | 780 | C | GLN | A | 112 | 22.970 | 36.399 | 52.192 | 1.00 | 58.29 | C |
| ATOM | 781 | O | GLN | A | 112 | 21.972 | 35.742 | 52.468 | 1.00 | 58.53 | O |
| ATOM | 782 | CB | GLN | A | 112 | 24.730 | 36.282 | 53.961 | 1.00 | 58.65 | C |
| ATOM | 783 | CG | GLN | A | 112 | 26.100 | 35.815 | 54.441 | 1.00 | 61.33 | C |
| ATOM | 784 | CD | GLN | A | 112 | 26.213 | 34.307 | 54.467 | 1.00 | 64.34 | C |
| ATOM | 785 | OE1 | GLN | A | 112 | 25.483 | 33.622 | 53.750 | 1.00 | 66.46 | O |
| ATOM | 786 | NE2 | GLN | A | 112 | 27.133 | 33.784 | 55.281 | 1.00 | 66.00 | N |
| ATOM | 787 | N | ASN | A | 113 | 22.919 | 37.581 | 51.580 | 1.00 | 58.45 | N |
| ATOM | 788 | CA | ASN | A | 113 | 21.653 | 38.222 | 51.240 | 1.00 | 58.79 | C |
| ATOM | 789 | C | ASN | A | 113 | 21.000 | 37.740 | 49.936 | 1.00 | 58.82 | C |
| ATOM | 790 | O | ASN | A | 113 | 19.971 | 38.284 | 49.536 | 1.00 | 59.69 | O |
| ATOM | 791 | CB | ASN | A | 113 | 21.813 | 39.759 | 51.171 | 1.00 | 58.81 | C |
| ATOM | 792 | CG | ASN | A | 113 | 22.160 | 40.387 | 52.525 | 1.00 | 59.17 | C |
| ATOM | 793 | OD1 | ASN | A | 113 | 21.863 | 39.824 | 53.593 | 1.00 | 57.49 | O |
| ATOM | 794 | ND2 | ASN | A | 113 | 22.786 | 41.567 | 52.482 | 1.00 | 58.34 | N |
| ATOM | 795 | N | PHE | A | 114 | 21.570 | 36.760 | 49.245 | 1.00 | 58.33 | N |
| ATOM | 796 | CA | PHE | A | 114 | 20.930 | 36.306 | 48.015 | 1.00 | 57.84 | C |
| ATOM | 797 | C | PHE | A | 114 | 19.922 | 35.220 | 48.334 | 1.00 | 57.57 | C |
| ATOM | 798 | O | PHE | A | 114 | 20.264 | 34.208 | 48.953 | 1.00 | 57.24 | O |
| ATOM | 799 | CB | PHE | A | 114 | 21.933 | 35.774 | 47.013 | 1.00 | 57.99 | C |
| ATOM | 800 | CG | PHE | A | 114 | 21.289 | 35.126 | 45.822 | 1.00 | 58.28 | C |
| ATOM | 801 | CD1 | PHE | A | 114 | 20.642 | 35.897 | 44.867 | 1.00 | 58.11 | C |
| ATOM | 802 | CD2 | PHE | A | 114 | 21.300 | 33.744 | 45.674 | 1.00 | 58.56 | C |
| ATOM | 803 | CE1 | PHE | A | 114 | 20.028 | 35.312 | 43.781 | 1.00 | 58.29 | C |
| ATOM | 804 | CE2 | PHE | A | 114 | 20.687 | 33.149 | 44.580 | 1.00 | 59.09 | C |
| ATOM | 805 | CZ | PHE | A | 114 | 20.050 | 33.937 | 43.630 | 1.00 | 58.80 | C |
| ATOM | 806 | N | LYS | A | 115 | 18.686 | 35.429 | 47.899 | 1.00 | 57.18 | N |
| ATOM | 807 | CA | LYS | A | 115 | 17.604 | 34.511 | 48.204 | 1.00 | 57.19 | C |
| ATOM | 808 | C | LYS | A | 115 | 17.037 | 33.942 | 46.903 | 1.00 | 57.17 | C |
| ATOM | 809 | O | LYS | A | 115 | 16.268 | 34.598 | 46.193 | 1.00 | 57.12 | O |
| ATOM | 810 | CB | LYS | A | 115 | 16.524 | 35.234 | 49.016 | 1.00 | 57.33 | C |
| ATOM | 811 | N | PRO | A | 116 | 17.384 | 32.699 | 46.610 | 1.00 | 56.97 | N |
| ATOM | 812 | CA | PRO | A | 116 | 17.042 | 32.097 | 45.319 | 1.00 | 57.01 | C |
| ATOM | 813 | C | PRO | A | 116 | 15.554 | 31.979 | 45.151 | 1.00 | 56.69 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 814 | O | PRO | A | 116 | 14.864 | 31.676 | 46.103 | 1.00 | 57.03 | O |
| ATOM | 815 | CB | PRO | A | 116 | 17.672 | 30.701 | 45.378 | 1.00 | 57.15 | C |
| ATOM | 816 | CG | PRO | A | 116 | 18.474 | 30.658 | 46.662 | 1.00 | 57.53 | C |
| ATOM | 817 | CD | PRO | A | 116 | 18.045 | 31.763 | 47.522 | 1.00 | 57.03 | C |
| ATOM | 818 | N | ARG | A | 117 | 15.073 | 32.212 | 43.945 | 1.00 | 56.65 | N |
| ATOM | 819 | CA | ARG | A | 117 | 13.663 | 32.087 | 43.656 | 1.00 | 56.39 | C |
| ATOM | 820 | C | ARG | A | 117 | 13.335 | 30.639 | 43.332 | 1.00 | 56.16 | C |
| ATOM | 821 | O | ARG | A | 117 | 12.160 | 30.272 | 43.279 | 1.00 | 56.65 | O |
| ATOM | 822 | CB | ARG | A | 117 | 13.280 | 32.971 | 42.508 | 1.00 | 56.56 | C |
| ATOM | 823 | N | SER | A | 118 | 14.350 | 29.810 | 43.110 | 1.00 | 55.25 | N |
| ATOM | 824 | CA | SER | A | 118 | 14.083 | 28.393 | 42.878 | 1.00 | 55.12 | C |
| ATOM | 825 | C | SER | A | 118 | 14.924 | 27.511 | 43.809 | 1.00 | 54.45 | C |
| ATOM | 826 | O | SER | A | 118 | 16.022 | 27.895 | 44.174 | 1.00 | 54.64 | O |
| ATOM | 827 | CB | SER | A | 118 | 14.322 | 28.029 | 41.415 | 1.00 | 54.89 | C |
| ATOM | 828 | OG | SER | A | 118 | 15.672 | 28.196 | 41.087 | 1.00 | 55.13 | O |
| ATOM | 829 | N | ASN | A | 119 | 14.381 | 26.362 | 44.211 | 1.00 | 53.66 | N |
| ATOM | 830 | CA | ASN | A | 119 | 15.089 | 25.412 | 45.060 | 1.00 | 53.43 | C |
| ATOM | 831 | C | ASN | A | 119 | 15.307 | 24.118 | 44.326 | 1.00 | 51.73 | C |
| ATOM | 832 | O | ASN | A | 119 | 14.472 | 23.705 | 43.552 | 1.00 | 51.23 | O |
| ATOM | 833 | CB | ASN | A | 119 | 14.277 | 25.063 | 46.311 | 1.00 | 54.32 | C |
| ATOM | 834 | CG | ASN | A | 119 | 13.711 | 26.272 | 46.994 | 1.00 | 57.18 | C |
| ATOM | 835 | OD1 | ASN | A | 119 | 14.448 | 27.099 | 47.563 | 1.00 | 60.84 | O |
| ATOM | 836 | ND2 | ASN | A | 119 | 12.384 | 26.384 | 46.964 | 1.00 | 61.01 | N |
| ATOM | 837 | N | ARG | A | 120 | 16.418 | 23.470 | 44.621 | 1.00 | 50.77 | N |
| ATOM | 838 | CA | ARG | A | 120 | 16.772 | 22.182 | 44.049 | 1.00 | 49.89 | C |
| ATOM | 839 | C | ARG | A | 120 | 16.388 | 21.062 | 44.999 | 1.00 | 49.87 | C |
| ATOM | 840 | O | ARG | A | 120 | 16.620 | 21.150 | 46.206 | 1.00 | 50.40 | O |
| ATOM | 841 | CB | ARG | A | 120 | 18.283 | 22.133 | 43.843 | 1.00 | 49.75 | C |
| ATOM | 842 | CG | ARG | A | 120 | 18.799 | 20.901 | 43.144 | 1.00 | 47.86 | C |
| ATOM | 843 | CD | ARG | A | 120 | 20.318 | 20.812 | 43.074 | 1.00 | 45.29 | C |
| ATOM | 844 | NE | ARG | A | 120 | 20.972 | 21.240 | 44.301 | 1.00 | 43.79 | N |
| ATOM | 845 | CZ | ARG | A | 120 | 21.316 | 20.432 | 45.314 | 1.00 | 43.05 | C |
| ATOM | 846 | NH1 | ARG | A | 120 | 21.053 | 19.126 | 45.277 | 1.00 | 40.07 | N |
| ATOM | 847 | NH2 | ARG | A | 120 | 21.921 | 20.942 | 46.379 | 1.00 | 41.03 | N |
| ATOM | 848 | N | GLU | A | 121 | 15.801 | 20.010 | 44.451 | 1.00 | 49.51 | N |
| ATOM | 849 | CA | GLU | A | 121 | 15.435 | 18.830 | 45.206 | 1.00 | 48.90 | C |
| ATOM | 850 | C | GLU | A | 121 | 15.905 | 17.609 | 44.411 | 1.00 | 47.95 | C |
| ATOM | 851 | O | GLU | A | 121 | 15.793 | 17.564 | 43.192 | 1.00 | 48.02 | O |
| ATOM | 852 | CB | GLU | A | 121 | 13.922 | 18.782 | 45.461 | 1.00 | 49.38 | C |
| ATOM | 853 | CG | GLU | A | 121 | 13.444 | 17.500 | 46.141 | 1.00 | 51.77 | C |
| ATOM | 854 | CD | GLU | A | 121 | 12.185 | 17.695 | 46.961 | 1.00 | 54.65 | C |
| ATOM | 855 | OE1 | GLU | A | 121 | 12.312 | 18.258 | 48.073 | 1.00 | 58.68 | O |
| ATOM | 856 | OE2 | GLU | A | 121 | 11.087 | 17.284 | 46.512 | 1.00 | 55.59 | O |
| ATOM | 857 | N | GLU | A | 122 | 16.455 | 16.622 | 45.104 | 1.00 | 47.05 | N |
| ATOM | 858 | CA | GLU | A | 122 | 16.938 | 15.423 | 44.463 | 1.00 | 46.05 | C |
| ATOM | 859 | C | GLU | A | 122 | 15.848 | 14.400 | 44.594 | 1.00 | 45.48 | C |
| ATOM | 860 | O | GLU | A | 122 | 15.313 | 14.220 | 45.666 | 1.00 | 45.63 | O |
| ATOM | 861 | CB | GLU | A | 122 | 18.200 | 14.940 | 45.158 | 1.00 | 45.67 | C |
| ATOM | 862 | CG | GLU | A | 122 | 19.346 | 15.921 | 45.063 | 1.00 | 44.97 | C |
| ATOM | 863 | CD | GLU | A | 122 | 19.789 | 16.154 | 43.623 | 1.00 | 45.49 | C |
| ATOM | 864 | OE1 | GLU | A | 122 | 19.985 | 15.144 | 42.902 | 1.00 | 44.79 | O |
| ATOM | 865 | OE2 | GLU | A | 122 | 19.925 | 17.337 | 43.207 | 1.00 | 42.47 | O |
| ATOM | 866 | N | MET | A | 123 | 15.481 | 13.751 | 43.503 | 1.00 | 44.95 | N |
| ATOM | 867 | CA | MET | A | 123 | 14.462 | 12.731 | 43.589 | 1.00 | 44.35 | C |
| ATOM | 868 | C | MET | A | 123 | 14.657 | 11.712 | 42.503 | 1.00 | 43.59 | C |
| ATOM | 869 | O | MET | A | 123 | 15.495 | 11.891 | 41.613 | 1.00 | 43.44 | O |
| ATOM | 870 | CB | MET | A | 123 | 13.078 | 13.358 | 43.490 | 1.00 | 44.59 | C |
| ATOM | 871 | CG | MET | A | 123 | 12.831 | 14.092 | 42.205 | 1.00 | 45.95 | C |
| ATOM | 872 | SD | MET | A | 123 | 11.244 | 14.946 | 42.206 | 1.00 | 47.99 | S |
| ATOM | 873 | CE | MET | A | 123 | 11.648 | 16.411 | 43.089 | 1.00 | 47.81 | C |
| ATOM | 874 | N | LYS | A | 124 | 13.880 | 10.638 | 42.603 | 1.00 | 42.37 | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 875 | CA | LYS | A | 124 | 13.869 | 9.575 | 41.623 | 1.00 | 41.47 | C |
| ATOM | 876 | C | LYS | A | 124 | 12.958 | 10.026 | 40.469 | 1.00 | 40.66 | C |
| ATOM | 877 | O | LYS | A | 124 | 12.066 | 10.862 | 40.654 | 1.00 | 39.80 | O |
| ATOM | 878 | CB | LYS | A | 124 | 13.354 | 8.267 | 42.250 | 1.00 | 41.45 | C |
| ATOM | 879 | CG | LYS | A | 124 | 14.160 | 7.756 | 43.470 | 1.00 | 41.70 | C |
| ATOM | 880 | CD | LYS | A | 124 | 15.574 | 7.301 | 43.076 | 1.00 | 42.20 | C |
| ATOM | 881 | CE | LYS | A | 124 | 16.451 | 6.989 | 44.273 | 1.00 | 41.37 | C |
| ATOM | 882 | NZ | LYS | A | 124 | 17.894 | 7.201 | 43.966 | 1.00 | 41.63 | N |
| ATOM | 883 | N | PHE | A | 125 | 13.178 | 9.460 | 39.284 | 1.00 | 39.69 | N |
| ATOM | 884 | CA | PHE | A | 125 | 12.463 | 9.889 | 38.101 | 1.00 | 38.95 | C |
| ATOM | 885 | C | PHE | A | 125 | 10.981 | 9.729 | 38.257 | 1.00 | 38.85 | C |
| ATOM | 886 | O | PHE | A | 125 | 10.217 | 10.613 | 37.890 | 1.00 | 37.81 | O |
| ATOM | 887 | CB | PHE | A | 125 | 12.942 | 9.154 | 36.862 | 1.00 | 38.45 | C |
| ATOM | 888 | CG | PHE | A | 125 | 12.618 | 9.871 | 35.610 | 1.00 | 39.49 | C |
| ATOM | 889 | CD1 | PHE | A | 125 | 13.471 | 10.840 | 35.118 | 1.00 | 40.78 | C |
| ATOM | 890 | CD2 | PHE | A | 125 | 11.428 | 9.655 | 34.967 | 1.00 | 40.81 | C |
| ATOM | 891 | CE1 | PHE | A | 125 | 13.181 | 11.530 | 33.992 | 1.00 | 40.48 | C |
| ATOM | 892 | CE2 | PHE | A | 125 | 11.123 | 10.353 | 33.825 | 1.00 | 41.39 | C |
| ATOM | 893 | CZ | PHE | A | 125 | 12.008 | 11.300 | 33.335 | 1.00 | 41.11 | C |
| ATOM | 894 | N | HIS | A | 126 | 10.575 | 8.602 | 38.835 | 1.00 | 39.49 | N |
| ATOM | 895 | CA | HIS | A | 126 | 9.161 | 8.342 | 39.044 | 1.00 | 39.91 | C |
| ATOM | 896 | C | HIS | A | 126 | 8.599 | 9.408 | 39.976 | 1.00 | 39.98 | C |
| ATOM | 897 | O | HIS | A | 126 | 7.455 | 9.821 | 39.830 | 1.00 | 39.26 | O |
| ATOM | 898 | CB | HIS | A | 126 | 8.906 | 6.899 | 39.552 | 1.00 | 40.45 | C |
| ATOM | 899 | CG | HIS | A | 126 | 9.034 | 6.727 | 41.033 | 1.00 | 41.06 | C |
| ATOM | 900 | ND1 | HIS | A | 126 | 7.987 | 6.950 | 41.899 | 1.00 | 40.98 | N |
| ATOM | 901 | CD2 | HIS | A | 126 | 10.092 | 6.367 | 41.801 | 1.00 | 41.92 | C |
| ATOM | 902 | CE1 | HIS | A | 126 | 8.403 | 6.759 | 43.140 | 1.00 | 43.22 | C |
| ATOM | 903 | NE2 | HIS | A | 126 | 9.676 | 6.405 | 43.108 | 1.00 | 42.45 | N |
| ATOM | 904 | N | GLU | A | 127 | 9.428 | 9.898 | 40.890 | 1.00 | 40.59 | N |
| ATOM | 905 | CA | GLU | A | 127 | 8.975 | 10.919 | 41.824 | 1.00 | 41.56 | C |
| ATOM | 906 | C | GLU | A | 127 | 8.749 | 12.213 | 41.062 | 1.00 | 41.66 | C |
| ATOM | 907 | O | GLU | A | 127 | 7.774 | 12.941 | 41.294 | 1.00 | 41.64 | O |
| ATOM | 908 | CB | GLU | A | 127 | 9.968 | 11.102 | 42.978 | 1.00 | 41.64 | C |
| ATOM | 909 | CG | GLU | A | 127 | 10.149 | 9.839 | 43.811 | 1.00 | 43.10 | C |
| ATOM | 910 | CD | GLU | A | 127 | 11.116 | 10.017 | 44.958 | 1.00 | 44.79 | C |
| ATOM | 911 | OE1 | GLU | A | 127 | 12.326 | 10.217 | 44.712 | 1.00 | 43.71 | O |
| ATOM | 912 | OE2 | GLU | A | 127 | 10.649 | 9.938 | 46.122 | 1.00 | 49.43 | O |
| ATOM | 913 | N | PHE | A | 128 | 9.636 | 12.491 | 40.124 | 1.00 | 41.96 | N |
| ATOM | 914 | CA | PHE | A | 128 | 9.504 | 13.705 | 39.337 | 1.00 | 41.99 | C |
| ATOM | 915 | C | PHE | A | 128 | 8.213 | 13.612 | 38.538 | 1.00 | 42.56 | C |
| ATOM | 916 | O | PHE | A | 128 | 7.400 | 14.537 | 38.507 | 1.00 | 41.93 | O |
| ATOM | 917 | CB | PHE | A | 128 | 10.708 | 13.864 | 38.416 | 1.00 | 41.57 | C |
| ATOM | 918 | CG | PHE | A | 128 | 10.470 | 14.795 | 37.244 | 1.00 | 41.38 | C |
| ATOM | 919 | CD1 | PHE | A | 128 | 10.199 | 16.136 | 37.449 | 1.00 | 39.65 | C |
| ATOM | 920 | CD2 | PHE | A | 128 | 10.537 | 14.330 | 35.950 | 1.00 | 39.22 | C |
| ATOM | 921 | CE1 | PHE | A | 128 | 9.980 | 16.975 | 36.399 | 1.00 | 40.36 | C |
| ATOM | 922 | CE2 | PHE | A | 128 | 10.329 | 15.191 | 34.888 | 1.00 | 41.57 | C |
| ATOM | 923 | CZ | PHE | A | 128 | 10.044 | 16.510 | 35.112 | 1.00 | 40.14 | C |
| ATOM | 924 | N | VAL | A | 129 | 7.999 | 12.463 | 37.921 | 1.00 | 43.85 | N |
| ATOM | 925 | CA | VAL | A | 129 | 6.813 | 12.288 | 37.095 | 1.00 | 44.87 | C |
| ATOM | 926 | C | VAL | A | 129 | 5.536 | 12.443 | 37.932 | 1.00 | 46.07 | C |
| ATOM | 927 | O | VAL | A | 129 | 4.574 | 13.093 | 37.505 | 1.00 | 45.32 | O |
| ATOM | 928 | CB | VAL | A | 129 | 6.798 | 10.920 | 36.425 | 1.00 | 44.99 | C |
| ATOM | 929 | CG1 | VAL | A | 129 | 5.496 | 10.725 | 35.631 | 1.00 | 44.81 | C |
| ATOM | 930 | CG2 | VAL | A | 129 | 8.030 | 10.718 | 35.550 | 1.00 | 43.96 | C |
| ATOM | 931 | N | GLU | A | 130 | 5.553 | 11.854 | 39.128 | 1.00 | 47.64 | N |
| ATOM | 932 | CA | GLU | A | 130 | 4.415 | 11.932 | 40.037 | 1.00 | 49.12 | C |
| ATOM | 933 | C | GLU | A | 130 | 4.136 | 13.390 | 40.384 | 1.00 | 49.48 | C |
| ATOM | 934 | O | GLU | A | 130 | 3.003 | 13.846 | 40.250 | 1.00 | 48.66 | O |
| ATOM | 935 | CB | GLU | A | 130 | 4.654 | 11.079 | 41.296 | 1.00 | 49.63 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 936 | CG | GLU | A | 130 | 4.534 | 9.576 | 41.062 | 1.00 | 50.81 | C |
| ATOM | 937 | CD | GLU | A | 130 | 5.257 | 8.747 | 42.117 | 1.00 | 53.77 | C |
| ATOM | 938 | OE1 | GLU | A | 130 | 5.566 | 9.295 | 43.204 | 1.00 | 55.27 | O |
| ATOM | 939 | OE2 | GLU | A | 130 | 5.518 | 7.543 | 41.856 | 1.00 | 54.73 | O |
| ATOM | 940 | N | LYS | A | 131 | 5.170 | 14.121 | 40.798 | 1.00 | 50.56 | N |
| ATOM | 941 | CA | LYS | A | 131 | 5.010 | 15.547 | 41.082 | 1.00 | 51.84 | C |
| ATOM | 942 | C | LYS | A | 131 | 4.385 | 16.276 | 39.886 | 1.00 | 52.55 | C |
| ATOM | 943 | O | LYS | A | 131 | 3.482 | 17.070 | 40.061 | 1.00 | 52.15 | O |
| ATOM | 944 | CB | LYS | A | 131 | 6.340 | 16.209 | 41.438 | 1.00 | 52.23 | C |
| ATOM | 945 | CG | LYS | A | 131 | 6.554 | 16.568 | 42.907 | 1.00 | 53.75 | C |
| ATOM | 946 | CD | LYS | A | 131 | 7.249 | 17.944 | 43.054 | 1.00 | 56.27 | C |
| ATOM | 947 | CE | LYS | A | 131 | 7.879 | 18.168 | 44.448 | 1.00 | 58.66 | C |
| ATOM | 948 | NZ | LYS | A | 131 | 8.247 | 19.628 | 44.725 | 1.00 | 59.31 | N |
| ATOM | 949 | N | LEU | A | 132 | 4.845 | 16.014 | 38.667 | 1.00 | 53.84 | N |
| ATOM | 950 | CA | LEU | A | 132 | 4.247 | 16.691 | 37.513 | 1.00 | 55.23 | C |
| ATOM | 951 | C | LEU | A | 132 | 2.762 | 16.408 | 37.407 | 1.00 | 55.96 | C |
| ATOM | 952 | O | LEU | A | 132 | 1.973 | 17.292 | 37.063 | 1.00 | 55.69 | O |
| ATOM | 953 | CB | LEU | A | 132 | 4.906 | 16.278 | 36.206 | 1.00 | 55.45 | C |
| ATOM | 954 | CG | LEU | A | 132 | 6.301 | 16.811 | 35.966 | 1.00 | 56.60 | C |
| ATOM | 955 | CD1 | LEU | A | 132 | 6.785 | 16.291 | 34.646 | 1.00 | 57.60 | C |
| ATOM | 956 | CD2 | LEU | A | 132 | 6.303 | 18.327 | 35.966 | 1.00 | 57.89 | C |
| ATOM | 957 | N | GLN | A | 133 | 2.397 | 15.157 | 37.669 | 1.00 | 57.19 | N |
| ATOM | 958 | CA | GLN | A | 133 | 0.998 | 14.739 | 37.663 | 1.00 | 58.15 | C |
| ATOM | 959 | C | GLN | A | 133 | 0.172 | 15.450 | 38.751 | 1.00 | 58.99 | C |
| ATOM | 960 | O | GLN | A | 133 | -0.915 | 15.950 | 38.470 | 1.00 | 58.73 | O |
| ATOM | 961 | CB | GLN | A | 133 | 0.897 | 13.230 | 37.824 | 1.00 | 58.03 | C |
| ATOM | 962 | N | ASP | A | 134 | 0.678 | 15.510 | 39.981 | 1.00 | 60.11 | N |
| ATOM | 963 | CA | ASP | A | 134 | -0.081 | 16.145 | 41.063 | 1.00 | 61.49 | C |
| ATOM | 964 | C | ASP | A | 134 | -0.362 | 17.629 | 40.783 | 1.00 | 61.55 | C |
| ATOM | 965 | O | ASP | A | 134 | -1.427 | 18.149 | 41.104 | 1.00 | 61.55 | O |
| ATOM | 966 | CB | ASP | A | 134 | 0.621 | 15.985 | 42.417 | 1.00 | 61.99 | C |
| ATOM | 967 | CG | ASP | A | 134 | -0.253 | 16.454 | 43.587 | 1.00 | 64.74 | C |
| ATOM | 968 | OD1 | ASP | A | 134 | -1.310 | 17.082 | 43.346 | 1.00 | 67.52 | O |
| ATOM | 969 | OD2 | ASP | A | 134 | 0.022 | 16.237 | 44.791 | 1.00 | 69.05 | O |
| ATOM | 970 | N | ILE | A | 135 | 0.594 | 18.312 | 40.179 | 1.00 | 61.80 | N |
| ATOM | 971 | CA | ILE | A | 135 | 0.402 | 19.706 | 39.860 | 1.00 | 62.08 | C |
| ATOM | 972 | C | ILE | A | 135 | -0.700 | 19.856 | 38.823 | 1.00 | 62.29 | C |
| ATOM | 973 | O | ILE | A | 135 | -1.639 | 20.620 | 39.013 | 1.00 | 61.91 | O |
| ATOM | 974 | CB | ILE | A | 135 | 1.711 | 20.301 | 39.366 | 1.00 | 62.21 | C |
| ATOM | 975 | CG1 | ILE | A | 135 | 2.705 | 20.391 | 40.528 | 1.00 | 62.47 | C |
| ATOM | 976 | CG2 | ILE | A | 135 | 1.478 | 21.670 | 38.783 | 1.00 | 62.19 | C |
| ATOM | 977 | CD1 | ILE | A | 135 | 4.157 | 20.437 | 40.100 | 1.00 | 62.96 | C |
| ATOM | 978 | N | GLN | A | 136 | -0.593 | 19.112 | 37.733 | 1.00 | 62.99 | N |
| ATOM | 979 | CA | GLN | A | 136 | -1.585 | 19.184 | 36.674 | 1.00 | 63.71 | C |
| ATOM | 980 | C | GLN | A | 136 | -2.977 | 18.992 | 37.259 | 1.00 | 64.44 | C |
| ATOM | 981 | O | GLN | A | 136 | -3.844 | 19.856 | 37.123 | 1.00 | 64.73 | O |
| ATOM | 982 | CB | GLN | A | 136 | -1.305 | 18.136 | 35.619 | 1.00 | 63.77 | C |
| ATOM | 983 | N | GLN | A | 137 | -3.170 | 17.871 | 37.948 | 1.00 | 65.12 | N |
| ATOM | 984 | CA | GLN | A | 137 | -4.472 | 17.509 | 38.497 | 1.00 | 65.60 | C |
| ATOM | 985 | C | GLN | A | 137 | -4.989 | 18.540 | 39.477 | 1.00 | 65.70 | C |
| ATOM | 986 | O | GLN | A | 137 | -6.175 | 18.871 | 39.447 | 1.00 | 66.17 | O |
| ATOM | 987 | CB | GLN | A | 137 | -4.421 | 16.117 | 39.161 | 1.00 | 65.72 | C |
| ATOM | 988 | N | ARG | A | 138 | -4.115 | 19.056 | 40.336 | 1.00 | 65.61 | N |
| ATOM | 989 | CA | ARG | A | 138 | -4.549 | 20.011 | 41.358 | 1.00 | 65.53 | C |
| ATOM | 990 | C | ARG | A | 138 | -4.578 | 21.441 | 40.823 | 1.00 | 64.96 | C |
| ATOM | 991 | O | ARG | A | 138 | -4.748 | 22.392 | 41.589 | 1.00 | 64.93 | O |
| ATOM | 992 | CB | ARG | A | 138 | -3.670 | 19.912 | 42.613 | 1.00 | 65.65 | C |
| ATOM | 993 | CG | ARG | A | 138 | -2.375 | 20.712 | 42.588 | 1.00 | 67.10 | C |
| ATOM | 994 | CD | ARG | A | 138 | -1.482 | 20.352 | 43.745 | 1.00 | 68.96 | C |
| ATOM | 995 | NE | ARG | A | 138 | -0.372 | 21.270 | 43.957 | 1.00 | 69.79 | N |
| ATOM | 996 | CZ | ARG | A | 138 | 0.905 | 20.919 | 43.880 | 1.00 | 71.69 | C |

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ATOM    997  NH1 ARG A 138       1.238  19.674  43.569  1.00 72.88           N
ATOM    998  NH2 ARG A 138       1.862  21.811  44.106  1.00 72.52           N
ATOM    999  N   GLY A 139      -4.426  21.593  39.508  1.00 64.31           N
ATOM   1000  CA  GLY A 139      -4.370  22.912  38.897  1.00 63.53           C
ATOM   1001  C   GLY A 139      -3.401  23.874  39.578  1.00 62.69           C
ATOM   1002  O   GLY A 139      -3.631  25.080  39.570  1.00 62.92           O
ATOM   1003  N   GLY A 140      -2.312  23.357  40.148  1.00 61.58           N
ATOM   1004  CA  GLY A 140      -1.345  24.183  40.861  1.00 60.52           C
ATOM   1005  C   GLY A 140      -0.539  25.103  39.958  1.00 59.56           C
ATOM   1006  O   GLY A 140      -0.449  24.867  38.748  1.00 59.45           O
ATOM   1007  N   GLU A 141       0.041  26.159  40.530  1.00 58.05           N
ATOM   1008  CA  GLU A 141       0.859  27.090  39.748  1.00 56.92           C
ATOM   1009  C   GLU A 141       2.366  26.751  39.832  1.00 54.97           C
ATOM   1010  O   GLU A 141       3.189  27.326  39.113  1.00 54.51           O
ATOM   1011  CB  GLU A 141       0.602  28.547  40.177  1.00 57.45           C
ATOM   1012  CG  GLU A 141      -0.707  29.171  39.680  1.00 59.67           C
ATOM   1013  CD  GLU A 141      -0.851  29.193  38.154  1.00 63.48           C
ATOM   1014  OE1 GLU A 141       0.179  29.107  37.436  1.00 65.30           O
ATOM   1015  OE2 GLU A 141      -2.007  29.298  37.664  1.00 66.13           O
ATOM   1016  N   GLU A 142       2.720  25.814  40.708  1.00 52.62           N
ATOM   1017  CA  GLU A 142       4.106  25.398  40.862  1.00 50.91           C
ATOM   1018  C   GLU A 142       4.679  24.958  39.516  1.00 48.93           C
ATOM   1019  O   GLU A 142       3.960  24.477  38.641  1.00 48.64           O
ATOM   1020  CB  GLU A 142       4.225  24.263  41.886  1.00 51.00           C
ATOM   1021  CG  GLU A 142       5.656  24.005  42.352  1.00 51.76           C
ATOM   1022  CD  GLU A 142       5.814  22.811  43.282  1.00 52.64           C
ATOM   1023  OE1 GLU A 142       4.871  22.009  43.447  1.00 55.52           O
ATOM   1024  OE2 GLU A 142       6.911  22.667  43.855  1.00 53.97           O
ATOM   1025  N   ARG A 143       5.979  25.139  39.356  1.00 46.58           N
ATOM   1026  CA  ARG A 143       6.652  24.751  38.133  1.00 45.12           C
ATOM   1027  C   ARG A 143       7.900  23.960  38.425  1.00 43.39           C
ATOM   1028  O   ARG A 143       8.616  24.242  39.387  1.00 43.58           O
ATOM   1029  CB  ARG A 143       7.069  25.983  37.360  1.00 45.52           C
ATOM   1030  CG  ARG A 143       5.943  26.747  36.729  1.00 45.38           C
ATOM   1031  CD  ARG A 143       6.488  27.899  35.969  1.00 46.06           C
ATOM   1032  NE  ARG A 143       5.473  28.649  35.252  1.00 45.33           N
ATOM   1033  CZ  ARG A 143       5.194  28.491  33.984  1.00 42.93           C
ATOM   1034  NH1 ARG A 143       5.836  27.573  33.253  1.00 41.86           N
ATOM   1035  NH2 ARG A 143       4.257  29.252  33.452  1.00 43.53           N
ATOM   1036  N   LEU A 144       8.182  22.991  37.578  1.00 41.08           N
ATOM   1037  CA  LEU A 144       9.337  22.163  37.784  1.00 39.63           C
ATOM   1038  C   LEU A 144      10.213  22.166  36.568  1.00 37.88           C
ATOM   1039  O   LEU A 144       9.734  22.249  35.444  1.00 36.26           O
ATOM   1040  CB  LEU A 144       8.889  20.727  38.018  1.00 40.26           C
ATOM   1041  CG  LEU A 144       7.974  20.529  39.223  1.00 41.73           C
ATOM   1042  CD1 LEU A 144       7.639  19.036  39.392  1.00 42.57           C
ATOM   1043  CD2 LEU A 144       8.585  21.102  40.503  1.00 41.42           C
ATOM   1044  N   TYR A 145      11.507  22.033  36.800  1.00 36.36           N
ATOM   1045  CA  TYR A 145      12.434  21.892  35.703  1.00 35.24           C
ATOM   1046  C   TYR A 145      13.485  20.862  36.107  1.00 34.89           C
ATOM   1047  O   TYR A 145      14.264  21.098  37.013  1.00 33.74           O
ATOM   1048  CB  TYR A 145      13.071  23.243  35.352  1.00 35.01           C
ATOM   1049  CG  TYR A 145      13.524  23.408  33.901  1.00 32.68           C
ATOM   1050  CD1 TYR A 145      13.817  22.324  33.099  1.00 30.20           C
ATOM   1051  CD2 TYR A 145      13.689  24.666  33.355  1.00 31.53           C
ATOM   1052  CE1 TYR A 145      14.237  22.493  31.762  1.00 29.87           C
ATOM   1053  CE2 TYR A 145      14.110  24.852  32.031  1.00 29.82           C
ATOM   1054  CZ  TYR A 145      14.373  23.765  31.228  1.00 30.06           C
ATOM   1055  OH  TYR A 145      14.789  23.953  29.897  1.00 28.17           O
ATOM   1056  N   LEU A 146      13.479  19.708  35.446  1.00 34.87           N
ATOM   1057  CA  LEU A 146      14.511  18.703  35.690  1.00 35.40           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1058 | C | LEU | A | 146 | 15.753 | 18.977 | 34.864 | 1.00 | 35.24 | C |
| ATOM | 1059 | O | LEU | A | 146 | 15.665 | 19.211 | 33.653 | 1.00 | 34.63 | O |
| ATOM | 1060 | CB | LEU | A | 146 | 14.008 | 17.312 | 35.358 | 1.00 | 35.79 | C |
| ATOM | 1061 | CG | LEU | A | 146 | 14.998 | 16.157 | 35.614 | 1.00 | 37.21 | C |
| ATOM | 1062 | CD1 | LEU | A | 146 | 14.221 | 14.918 | 35.969 | 1.00 | 36.28 | C |
| ATOM | 1063 | CD2 | LEU | A | 146 | 15.907 | 15.872 | 34.399 | 1.00 | 38.78 | C |
| ATOM | 1064 | N | GLN | A | 147 | 16.907 | 18.883 | 35.515 | 1.00 | 34.82 | N |
| ATOM | 1065 | CA | GLN | A | 147 | 18.179 | 19.206 | 34.884 | 1.00 | 35.00 | C |
| ATOM | 1066 | C | GLN | A | 147 | 19.222 | 18.341 | 35.525 | 1.00 | 34.90 | C |
| ATOM | 1067 | O | GLN | A | 147 | 19.626 | 18.568 | 36.664 | 1.00 | 35.65 | O |
| ATOM | 1068 | CB | GLN | A | 147 | 18.526 | 20.679 | 35.078 | 1.00 | 35.09 | C |
| ATOM | 1069 | CG | GLN | A | 147 | 17.392 | 21.636 | 34.720 | 1.00 | 35.83 | C |
| ATOM | 1070 | CD | GLN | A | 147 | 17.848 | 23.085 | 34.706 | 1.00 | 36.90 | C |
| ATOM | 1071 | OE1 | GLN | A | 147 | 17.091 | 23.961 | 34.302 | 1.00 | 39.61 | O |
| ATOM | 1072 | NE2 | GLN | A | 147 | 19.088 | 23.336 | 35.126 | 1.00 | 35.05 | N |
| ATOM | 1073 | N | GLN | A | 148 | 19.673 | 17.358 | 34.773 | 1.00 | 35.00 | N |
| ATOM | 1074 | CA | GLN | A | 148 | 20.492 | 16.300 | 35.294 | 1.00 | 34.89 | C |
| ATOM | 1075 | C | GLN | A | 148 | 21.376 | 15.709 | 34.255 | 1.00 | 35.35 | C |
| ATOM | 1076 | O | GLN | A | 148 | 20.941 | 15.318 | 33.181 | 1.00 | 35.25 | O |
| ATOM | 1077 | CB | GLN | A | 148 | 19.580 | 15.186 | 35.791 | 1.00 | 35.27 | C |
| ATOM | 1078 | CG | GLN | A | 148 | 20.335 | 13.914 | 36.269 | 1.00 | 35.11 | C |
| ATOM | 1079 | CD | GLN | A | 148 | 21.317 | 14.230 | 37.389 | 1.00 | 34.12 | C |
| ATOM | 1080 | OE1 | GLN | A | 148 | 20.998 | 15.033 | 38.277 | 1.00 | 33.18 | O |
| ATOM | 1081 | NE2 | GLN | A | 148 | 22.521 | 13.652 | 37.324 | 1.00 | 30.47 | N |
| ATOM | 1082 | N | THR | A | 149 | 22.631 | 15.641 | 34.600 | 1.00 | 36.56 | N |
| ATOM | 1083 | CA | THR | A | 149 | 23.648 | 15.088 | 33.754 | 1.00 | 38.26 | C |
| ATOM | 1084 | C | THR | A | 149 | 23.394 | 13.609 | 33.615 | 1.00 | 38.31 | C |
| ATOM | 1085 | O | THR | A | 149 | 23.068 | 12.956 | 34.597 | 1.00 | 38.70 | O |
| ATOM | 1086 | CB | THR | A | 149 | 24.992 | 15.362 | 34.463 | 1.00 | 38.76 | C |
| ATOM | 1087 | OG1 | THR | A | 149 | 25.290 | 16.747 | 34.277 | 1.00 | 41.68 | O |
| ATOM | 1088 | CG2 | THR | A | 149 | 26.139 | 14.710 | 33.797 | 1.00 | 40.77 | C |
| ATOM | 1089 | N | LEU | A | 150 | 23.516 | 13.087 | 32.399 | 1.00 | 38.77 | N |
| ATOM | 1090 | CA | LEU | A | 150 | 23.373 | 11.664 | 32.149 | 1.00 | 39.27 | C |
| ATOM | 1091 | C | LEU | A | 150 | 24.604 | 10.898 | 32.679 | 1.00 | 39.85 | C |
| ATOM | 1092 | O | LEU | A | 150 | 25.733 | 11.207 | 32.321 | 1.00 | 39.99 | O |
| ATOM | 1093 | CB | LEU | A | 150 | 23.220 | 11.402 | 30.660 | 1.00 | 39.15 | C |
| ATOM | 1094 | CG | LEU | A | 150 | 21.943 | 11.860 | 29.962 | 1.00 | 40.72 | C |
| ATOM | 1095 | CD1 | LEU | A | 150 | 22.058 | 11.673 | 28.459 | 1.00 | 41.91 | C |
| ATOM | 1096 | CD2 | LEU | A | 150 | 20.764 | 11.106 | 30.458 | 1.00 | 41.30 | C |
| ATOM | 1097 | N | ASN | A | 151 | 24.392 | 9.898 | 33.526 | 1.00 | 40.26 | N |
| ATOM | 1098 | CA | ASN | A | 151 | 25.510 | 9.124 | 34.062 | 1.00 | 40.90 | C |
| ATOM | 1099 | C | ASN | A | 151 | 25.291 | 7.607 | 34.041 | 1.00 | 41.95 | C |
| ATOM | 1100 | O | ASN | A | 151 | 24.327 | 7.098 | 33.441 | 1.00 | 41.72 | O |
| ATOM | 1101 | CB | ASN | A | 151 | 25.778 | 9.575 | 35.489 | 1.00 | 40.77 | C |
| ATOM | 1102 | CG | ASN | A | 151 | 24.564 | 9.439 | 36.349 | 1.00 | 39.85 | C |
| ATOM | 1103 | OD1 | ASN | A | 151 | 24.002 | 8.340 | 36.483 | 1.00 | 37.92 | O |
| ATOM | 1104 | ND2 | ASN | A | 151 | 24.107 | 10.558 | 36.897 | 1.00 | 36.89 | N |
| ATOM | 1105 | N | ASP | A | 152 | 26.176 | 6.894 | 34.735 | 1.00 | 42.89 | N |
| ATOM | 1106 | CA | ASP | A | 152 | 26.175 | 5.431 | 34.756 | 1.00 | 43.75 | C |
| ATOM | 1107 | C | ASP | A | 152 | 24.950 | 4.768 | 35.272 | 1.00 | 43.37 | C |
| ATOM | 1108 | O | ASP | A | 152 | 24.787 | 3.581 | 35.052 | 1.00 | 43.66 | O |
| ATOM | 1109 | CB | ASP | A | 152 | 27.256 | 4.895 | 35.695 | 1.00 | 44.77 | C |
| ATOM | 1110 | CG | ASP | A | 152 | 28.539 | 5.555 | 35.500 | 1.00 | 48.22 | C |
| ATOM | 1111 | OD1 | ASP | A | 152 | 28.835 | 5.881 | 34.325 | 1.00 | 57.47 | O |
| ATOM | 1112 | OD2 | ASP | A | 152 | 29.291 | 5.826 | 36.437 | 1.00 | 51.28 | O |
| ATOM | 1113 | N | THR | A | 153 | 24.119 | 5.466 | 36.025 | 1.00 | 43.41 | N |
| ATOM | 1114 | CA | THR | A | 153 | 22.983 | 4.783 | 36.631 | 1.00 | 43.38 | C |
| ATOM | 1115 | C | THR | A | 153 | 21.820 | 4.605 | 35.676 | 1.00 | 42.99 | C |
| ATOM | 1116 | O | THR | A | 153 | 20.866 | 3.945 | 36.012 | 1.00 | 43.44 | O |
| ATOM | 1117 | CB | THR | A | 153 | 22.489 | 5.507 | 37.875 | 1.00 | 43.44 | C |
| ATOM | 1118 | OG1 | THR | A | 153 | 21.749 | 6.678 | 37.499 | 1.00 | 46.09 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1119 | CG2 | THR | A | 153 | 23.651 | 6.008 | 38.725 | 1.00 | 42.99 | C |
| ATOM | 1120 | N | VAL | A | 154 | 21.874 | 5.185 | 34.491 | 1.00 | 42.88 | N |
| ATOM | 1121 | CA | VAL | A | 154 | 20.757 | 5.015 | 33.572 | 1.00 | 42.71 | C |
| ATOM | 1122 | C | VAL | A | 154 | 20.700 | 3.563 | 33.177 | 1.00 | 42.42 | C |
| ATOM | 1123 | O | VAL | A | 154 | 21.729 | 2.892 | 33.193 | 1.00 | 42.39 | O |
| ATOM | 1124 | CB | VAL | A | 154 | 20.889 | 5.875 | 32.300 | 1.00 | 42.67 | C |
| ATOM | 1125 | CG1 | VAL | A | 154 | 20.857 | 7.347 | 32.660 | 1.00 | 43.04 | C |
| ATOM | 1126 | CG2 | VAL | A | 154 | 22.159 | 5.516 | 31.538 | 1.00 | 42.56 | C |
| ATOM | 1127 | N | GLY | A | 155 | 19.502 | 3.097 | 32.814 | 1.00 | 42.11 | N |
| ATOM | 1128 | CA | GLY | A | 155 | 19.261 | 1.725 | 32.411 | 1.00 | 41.52 | C |
| ATOM | 1129 | C | GLY | A | 155 | 19.642 | 1.317 | 30.992 | 1.00 | 41.85 | C |
| ATOM | 1130 | O | GLY | A | 155 | 19.977 | 2.140 | 30.123 | 1.00 | 41.87 | O |
| ATOM | 1131 | N | ARG | A | 156 | 19.512 | 0.012 | 30.750 | 1.00 | 41.36 | N |
| ATOM | 1132 | CA | ARG | A | 156 | 19.961 | -0.623 | 29.511 | 1.00 | 40.88 | C |
| ATOM | 1133 | C | ARG | A | 156 | 19.397 | -0.005 | 28.247 | 1.00 | 40.03 | C |
| ATOM | 1134 | O | ARG | A | 156 | 20.135 | 0.304 | 27.339 | 1.00 | 40.36 | O |
| ATOM | 1135 | CB | ARG | A | 156 | 19.670 | -2.148 | 29.555 | 1.00 | 40.77 | C |
| ATOM | 1136 | N | LYS | A | 157 | 18.090 | 0.146 | 28.181 | 1.00 | 39.16 | N |
| ATOM | 1137 | CA | LYS | A | 157 | 17.503 | 0.697 | 26.990 | 1.00 | 38.81 | C |
| ATOM | 1138 | C | LYS | A | 157 | 18.078 | 2.114 | 26.738 | 1.00 | 38.38 | C |
| ATOM | 1139 | O | LYS | A | 157 | 18.363 | 2.464 | 25.594 | 1.00 | 37.97 | O |
| ATOM | 1140 | CB | LYS | A | 157 | 15.968 | 0.714 | 27.090 | 1.00 | 39.20 | C |
| ATOM | 1141 | CG | LYS | A | 157 | 15.266 | -0.575 | 26.642 | 1.00 | 36.80 | C |
| ATOM | 1142 | N | ILE | A | 158 | 18.268 | 2.909 | 27.791 | 1.00 | 37.56 | N |
| ATOM | 1143 | CA | ILE | A | 158 | 18.759 | 4.287 | 27.606 | 1.00 | 37.28 | C |
| ATOM | 1144 | C | ILE | A | 158 | 20.180 | 4.281 | 27.126 | 1.00 | 37.22 | C |
| ATOM | 1145 | O | ILE | A | 158 | 20.582 | 5.120 | 26.302 | 1.00 | 37.08 | O |
| ATOM | 1146 | CB | ILE | A | 158 | 18.692 | 5.101 | 28.882 | 1.00 | 36.72 | C |
| ATOM | 1147 | CG1 | ILE | A | 158 | 17.257 | 5.220 | 29.356 | 1.00 | 37.17 | C |
| ATOM | 1148 | CG2 | ILE | A | 158 | 19.254 | 6.465 | 28.646 | 1.00 | 36.48 | C |
| ATOM | 1149 | CD1 | ILE | A | 158 | 16.359 | 5.900 | 28.409 | 1.00 | 38.28 | C |
| ATOM | 1150 | N | VAL | A | 159 | 20.934 | 3.335 | 27.655 | 1.00 | 36.85 | N |
| ATOM | 1151 | CA | VAL | A | 159 | 22.319 | 3.177 | 27.284 | 1.00 | 37.05 | C |
| ATOM | 1152 | C | VAL | A | 159 | 22.349 | 2.864 | 25.785 | 1.00 | 36.45 | C |
| ATOM | 1153 | O | VAL | A | 159 | 23.165 | 3.410 | 25.057 | 1.00 | 35.81 | O |
| ATOM | 1154 | CB | VAL | A | 159 | 22.988 | 2.042 | 28.096 | 1.00 | 37.36 | C |
| ATOM | 1155 | CG1 | VAL | A | 159 | 24.248 | 1.567 | 27.427 | 1.00 | 38.43 | C |
| ATOM | 1156 | CG2 | VAL | A | 159 | 23.302 | 2.499 | 29.494 | 1.00 | 37.81 | C |
| ATOM | 1157 | N | MET | A | 160 | 21.453 | 1.990 | 25.339 | 1.00 | 35.84 | N |
| ATOM | 1158 | CA | MET | A | 160 | 21.369 | 1.637 | 23.910 | 1.00 | 36.30 | C |
| ATOM | 1159 | C | MET | A | 160 | 21.064 | 2.883 | 23.074 | 1.00 | 34.46 | C |
| ATOM | 1160 | O | MET | A | 160 | 21.715 | 3.142 | 22.083 | 1.00 | 33.88 | O |
| ATOM | 1161 | CB | MET | A | 160 | 20.294 | 0.576 | 23.656 | 1.00 | 36.83 | C |
| ATOM | 1162 | CG | MET | A | 160 | 20.654 | -0.763 | 24.225 | 1.00 | 39.89 | C |
| ATOM | 1163 | SD | MET | A | 160 | 21.916 | -1.579 | 23.249 | 1.00 | 46.87 | S |
| ATOM | 1164 | CE | MET | A | 160 | 21.005 | -1.940 | 21.669 | 1.00 | 47.08 | C |
| ATOM | 1165 | N | ASP | A | 161 | 20.078 | 3.648 | 23.505 | 1.00 | 33.13 | N |
| ATOM | 1166 | CA | ASP | A | 161 | 19.732 | 4.901 | 22.857 | 1.00 | 32.80 | C |
| ATOM | 1167 | C | ASP | A | 161 | 20.931 | 5.877 | 22.747 | 1.00 | 31.75 | C |
| ATOM | 1168 | O | ASP | A | 161 | 21.209 | 6.425 | 21.691 | 1.00 | 31.06 | O |
| ATOM | 1169 | CB | ASP | A | 161 | 18.598 | 5.553 | 23.631 | 1.00 | 32.93 | C |
| ATOM | 1170 | CG | ASP | A | 161 | 17.278 | 4.822 | 23.473 | 1.00 | 33.90 | C |
| ATOM | 1171 | OD1 | ASP | A | 161 | 17.148 | 3.961 | 22.568 | 1.00 | 28.71 | O |
| ATOM | 1172 | OD2 | ASP | A | 161 | 16.301 | 5.064 | 24.226 | 1.00 | 38.17 | O |
| ATOM | 1173 | N | PHE | A | 162 | 21.646 | 6.052 | 23.849 | 1.00 | 31.05 | N |
| ATOM | 1174 | CA | PHE | A | 162 | 22.763 | 6.968 | 23.930 | 1.00 | 30.52 | C |
| ATOM | 1175 | C | PHE | A | 162 | 23.835 | 6.553 | 22.979 | 1.00 | 28.89 | C |
| ATOM | 1176 | O | PHE | A | 162 | 24.477 | 7.369 | 22.371 | 1.00 | 29.43 | O |
| ATOM | 1177 | CB | PHE | A | 162 | 23.311 | 6.948 | 25.375 | 1.00 | 30.80 | C |
| ATOM | 1178 | CG | PHE | A | 162 | 24.493 | 7.839 | 25.617 | 1.00 | 31.81 | C |
| ATOM | 1179 | CD1 | PHE | A | 162 | 24.325 | 9.179 | 25.904 | 1.00 | 35.81 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1180 | CD2 | PHE | A | 162 | 25.770 | 7.322 | 25.653 | 1.00 | 35.00 | C |
| ATOM | 1181 | CE1 | PHE | A | 162 | 25.430 | 10.000 | 26.197 | 1.00 | 35.94 | C |
| ATOM | 1182 | CE2 | PHE | A | 162 | 26.887 | 8.143 | 25.941 | 1.00 | 35.90 | C |
| ATOM | 1183 | CZ | PHE | A | 162 | 26.711 | 9.467 | 26.202 | 1.00 | 35.61 | C |
| ATOM | 1184 | N | LEU | A | 163 | 24.067 | 5.271 | 22.914 | 1.00 | 28.19 | N |
| ATOM | 1185 | CA | LEU | A | 163 | 25.103 | 4.728 | 22.065 | 1.00 | 28.08 | C |
| ATOM | 1186 | C | LEU | A | 163 | 24.735 | 4.923 | 20.590 | 1.00 | 27.13 | C |
| ATOM | 1187 | O | LEU | A | 163 | 25.603 | 4.973 | 19.751 | 1.00 | 26.83 | O |
| ATOM | 1188 | CB | LEU | A | 163 | 25.306 | 3.244 | 22.368 | 1.00 | 27.86 | C |
| ATOM | 1189 | CG | LEU | A | 163 | 26.137 | 2.987 | 23.604 | 1.00 | 28.73 | C |
| ATOM | 1190 | CD1 | LEU | A | 163 | 26.180 | 1.512 | 23.849 | 1.00 | 29.77 | C |
| ATOM | 1191 | CD2 | LEU | A | 163 | 27.559 | 3.522 | 23.464 | 1.00 | 29.70 | C |
| ATOM | 1192 | N | GLY | A | 164 | 23.448 | 4.998 | 20.303 | 1.00 | 26.50 | N |
| ATOM | 1193 | CA | GLY | A | 164 | 22.956 | 5.244 | 18.959 | 1.00 | 27.37 | C |
| ATOM | 1194 | C | GLY | A | 164 | 22.949 | 6.712 | 18.493 | 1.00 | 27.88 | C |
| ATOM | 1195 | O | GLY | A | 164 | 22.483 | 6.988 | 17.365 | 1.00 | 28.42 | O |
| ATOM | 1196 | N | PHE | A | 165 | 23.420 | 7.635 | 19.344 | 1.00 | 26.36 | N |
| ATOM | 1197 | CA | PHE | A | 165 | 23.530 | 9.011 | 18.958 | 1.00 | 26.57 | C |
| ATOM | 1198 | C | PHE | A | 165 | 24.540 | 9.052 | 17.820 | 1.00 | 26.12 | C |
| ATOM | 1199 | O | PHE | A | 165 | 25.381 | 8.202 | 17.756 | 1.00 | 24.23 | O |
| ATOM | 1200 | CB | PHE | A | 165 | 24.024 | 9.867 | 20.153 | 1.00 | 26.86 | C |
| ATOM | 1201 | CG | PHE | A | 165 | 22.979 | 10.070 | 21.252 | 1.00 | 27.80 | C |
| ATOM | 1202 | CD1 | PHE | A | 165 | 21.701 | 9.533 | 21.144 | 1.00 | 27.80 | C |
| ATOM | 1203 | CD2 | PHE | A | 165 | 23.274 | 10.820 | 22.367 | 1.00 | 28.58 | C |
| ATOM | 1204 | CE1 | PHE | A | 165 | 20.765 | 9.744 | 22.117 | 1.00 | 26.89 | C |
| ATOM | 1205 | CE2 | PHE | A | 165 | 22.329 | 11.042 | 23.364 | 1.00 | 28.45 | C |
| ATOM | 1206 | CZ | PHE | A | 165 | 21.086 | 10.504 | 23.243 | 1.00 | 28.78 | C |
| ATOM | 1207 | N | ASN | A | 166 | 24.496 | 10.077 | 16.963 | 1.00 | 26.15 | N |
| ATOM | 1208 | CA | ASN | A | 166 | 25.441 | 10.165 | 15.837 | 1.00 | 25.91 | C |
| ATOM | 1209 | C | ASN | A | 166 | 26.861 | 10.675 | 16.226 | 1.00 | 26.12 | C |
| ATOM | 1210 | O | ASN | A | 166 | 27.288 | 11.793 | 15.894 | 1.00 | 25.48 | O |
| ATOM | 1211 | CB | ASN | A | 166 | 24.834 | 11.004 | 14.705 | 1.00 | 25.51 | C |
| ATOM | 1212 | CG | ASN | A | 166 | 25.634 | 10.916 | 13.431 | 1.00 | 24.43 | C |
| ATOM | 1213 | OD1 | ASN | A | 166 | 26.751 | 10.323 | 13.429 | 1.00 | 23.40 | O |
| ATOM | 1214 | ND2 | ASN | A | 166 | 25.078 | 11.479 | 12.318 | 1.00 | 17.22 | N |
| ATOM | 1215 | N | TRP | A | 167 | 27.566 | 9.817 | 16.940 | 1.00 | 26.11 | N |
| ATOM | 1216 | CA | TRP | A | 167 | 28.907 | 10.080 | 17.401 | 1.00 | 26.58 | C |
| ATOM | 1217 | C | TRP | A | 167 | 29.817 | 10.336 | 16.206 | 1.00 | 27.07 | C |
| ATOM | 1218 | O | TRP | A | 167 | 30.737 | 11.139 | 16.252 | 1.00 | 26.92 | O |
| ATOM | 1219 | CB | TRP | A | 167 | 29.389 | 8.860 | 18.249 | 1.00 | 26.02 | C |
| ATOM | 1220 | CG | TRP | A | 167 | 28.537 | 8.750 | 19.498 | 1.00 | 27.18 | C |
| ATOM | 1221 | CD1 | TRP | A | 167 | 27.620 | 7.784 | 19.809 | 1.00 | 28.08 | C |
| ATOM | 1222 | CD2 | TRP | A | 167 | 28.452 | 9.719 | 20.550 | 1.00 | 27.33 | C |
| ATOM | 1223 | NE1 | TRP | A | 167 | 27.013 | 8.071 | 21.013 | 1.00 | 27.87 | N |
| ATOM | 1224 | CE2 | TRP | A | 167 | 27.503 | 9.254 | 21.481 | 1.00 | 26.46 | C |
| ATOM | 1225 | CE3 | TRP | A | 167 | 29.103 | 10.929 | 20.804 | 1.00 | 26.22 | C |
| ATOM | 1226 | CZ2 | TRP | A | 167 | 27.180 | 9.951 | 22.622 | 1.00 | 28.27 | C |
| ATOM | 1227 | CZ3 | TRP | A | 167 | 28.784 | 11.615 | 21.920 | 1.00 | 27.56 | C |
| ATOM | 1228 | CH2 | TRP | A | 167 | 27.821 | 11.128 | 22.833 | 1.00 | 28.04 | C |
| ATOM | 1229 | N | ASN | A | 168 | 29.585 | 9.632 | 15.114 | 1.00 | 27.98 | N |
| ATOM | 1230 | CA | ASN | A | 168 | 30.430 | 9.833 | 13.959 | 1.00 | 28.32 | C |
| ATOM | 1231 | C | ASN | A | 168 | 30.470 | 11.319 | 13.573 | 1.00 | 29.00 | C |
| ATOM | 1232 | O | ASN | A | 168 | 31.547 | 11.894 | 13.390 | 1.00 | 30.41 | O |
| ATOM | 1233 | CB | ASN | A | 168 | 29.909 | 9.018 | 12.812 | 1.00 | 28.58 | C |
| ATOM | 1234 | CG | ASN | A | 168 | 30.758 | 9.145 | 11.570 | 1.00 | 29.28 | C |
| ATOM | 1235 | OD1 | ASN | A | 168 | 31.899 | 8.739 | 11.579 | 1.00 | 30.27 | O |
| ATOM | 1236 | ND2 | ASN | A | 168 | 30.186 | 9.677 | 10.487 | 1.00 | 28.46 | N |
| ATOM | 1237 | N | TRP | A | 169 | 29.301 | 11.942 | 13.462 | 1.00 | 27.93 | N |
| ATOM | 1238 | CA | TRP | A | 169 | 29.228 | 13.343 | 13.074 | 1.00 | 27.25 | C |
| ATOM | 1239 | C | TRP | A | 169 | 29.726 | 14.266 | 14.179 | 1.00 | 27.20 | C |
| ATOM | 1240 | O | TRP | A | 169 | 30.444 | 15.224 | 13.925 | 1.00 | 26.30 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1241 | CB | TRP | A | 169 | 27.777 | 13.734 | 12.691 | 1.00 | 26.63 | C |
| ATOM | 1242 | CG | TRP | A | 169 | 27.615 | 15.168 | 12.355 | 1.00 | 25.15 | C |
| ATOM | 1243 | CD1 | TRP | A | 169 | 27.804 | 15.745 | 11.130 | 1.00 | 24.89 | C |
| ATOM | 1244 | CD2 | TRP | A | 169 | 27.261 | 16.229 | 13.237 | 1.00 | 23.66 | C |
| ATOM | 1245 | NE1 | TRP | A | 169 | 27.591 | 17.095 | 11.195 | 1.00 | 22.98 | N |
| ATOM | 1246 | CE2 | TRP | A | 169 | 27.257 | 17.427 | 12.476 | 1.00 | 25.81 | C |
| ATOM | 1247 | CE3 | TRP | A | 169 | 26.927 | 16.292 | 14.576 | 1.00 | 24.44 | C |
| ATOM | 1248 | CZ2 | TRP | A | 169 | 26.933 | 18.680 | 13.018 | 1.00 | 26.96 | C |
| ATOM | 1249 | CZ3 | TRP | A | 169 | 26.624 | 17.525 | 15.127 | 1.00 | 28.68 | C |
| ATOM | 1250 | CH2 | TRP | A | 169 | 26.611 | 18.710 | 14.336 | 1.00 | 28.73 | C |
| ATOM | 1251 | N | ILE | A | 170 | 29.323 | 14.026 | 15.409 | 1.00 | 27.29 | N |
| ATOM | 1252 | CA | ILE | A | 170 | 29.725 | 14.985 | 16.406 | 1.00 | 28.36 | C |
| ATOM | 1253 | C | ILE | A | 170 | 31.252 | 14.874 | 16.686 | 1.00 | 29.15 | C |
| ATOM | 1254 | O | ILE | A | 170 | 31.920 | 15.875 | 16.866 | 1.00 | 29.81 | O |
| ATOM | 1255 | CB | ILE | A | 170 | 28.814 | 14.947 | 17.672 | 1.00 | 28.10 | C |
| ATOM | 1256 | CG1 | ILE | A | 170 | 28.882 | 16.277 | 18.386 | 1.00 | 26.98 | C |
| ATOM | 1257 | CG2 | ILE | A | 170 | 29.198 | 13.838 | 18.593 | 1.00 | 27.15 | C |
| ATOM | 1258 | CD1 | ILE | A | 170 | 27.855 | 16.400 | 19.530 | 1.00 | 28.88 | C |
| ATOM | 1259 | N | ASN | A | 171 | 31.809 | 13.679 | 16.653 | 1.00 | 29.35 | N |
| ATOM | 1260 | CA | ASN | A | 171 | 33.261 | 13.535 | 16.843 | 1.00 | 30.18 | C |
| ATOM | 1261 | C | ASN | A | 171 | 34.060 | 14.259 | 15.752 | 1.00 | 30.67 | C |
| ATOM | 1262 | O | ASN | A | 171 | 35.117 | 14.823 | 16.036 | 1.00 | 31.32 | O |
| ATOM | 1263 | CB | ASN | A | 171 | 33.705 | 12.058 | 16.861 | 1.00 | 29.80 | C |
| ATOM | 1264 | CG | ASN | A | 171 | 33.210 | 11.274 | 18.094 | 1.00 | 30.17 | C |
| ATOM | 1265 | OD1 | ASN | A | 171 | 32.682 | 11.821 | 19.051 | 1.00 | 30.65 | O |
| ATOM | 1266 | ND2 | ASN | A | 171 | 33.372 | 9.968 | 18.036 | 1.00 | 31.44 | N |
| ATOM | 1267 | N | LYS | A | 172 | 33.591 | 14.231 | 14.509 | 1.00 | 30.94 | N |
| ATOM | 1268 | CA | LYS | A | 172 | 34.297 | 14.960 | 13.461 | 1.00 | 32.29 | C |
| ATOM | 1269 | C | LYS | A | 172 | 34.211 | 16.473 | 13.755 | 1.00 | 31.79 | C |
| ATOM | 1270 | O | LYS | A | 172 | 35.128 | 17.234 | 13.482 | 1.00 | 32.06 | O |
| ATOM | 1271 | CB | LYS | A | 172 | 33.754 | 14.646 | 12.055 | 1.00 | 32.47 | C |
| ATOM | 1272 | CG | LYS | A | 172 | 34.168 | 13.298 | 11.539 | 1.00 | 36.36 | C |
| ATOM | 1273 | CD | LYS | A | 172 | 33.697 | 13.012 | 10.072 | 1.00 | 41.05 | C |
| ATOM | 1274 | CE | LYS | A | 172 | 34.338 | 11.721 | 9.543 | 1.00 | 44.14 | C |
| ATOM | 1275 | NZ | LYS | A | 172 | 34.321 | 11.571 | 8.024 | 1.00 | 49.11 | N |
| ATOM | 1276 | N | GLN | A | 173 | 33.099 | 16.900 | 14.316 | 1.00 | 31.59 | N |
| ATOM | 1277 | CA | GLN | A | 173 | 32.931 | 18.299 | 14.616 | 1.00 | 31.80 | C |
| ATOM | 1278 | C | GLN | A | 173 | 33.965 | 18.680 | 15.681 | 1.00 | 32.04 | C |
| ATOM | 1279 | O | GLN | A | 173 | 34.670 | 19.687 | 15.534 | 1.00 | 32.67 | O |
| ATOM | 1280 | CB | GLN | A | 173 | 31.522 | 18.581 | 15.117 | 1.00 | 31.45 | C |
| ATOM | 1281 | CG | GLN | A | 173 | 30.477 | 18.685 | 14.067 | 1.00 | 31.68 | C |
| ATOM | 1282 | CD | GLN | A | 173 | 30.782 | 19.751 | 13.050 | 1.00 | 32.76 | C |
| ATOM | 1283 | OE1 | GLN | A | 173 | 31.198 | 20.852 | 13.405 | 1.00 | 36.55 | O |
| ATOM | 1284 | NE2 | GLN | A | 173 | 30.583 | 19.440 | 11.790 | 1.00 | 32.28 | N |
| ATOM | 1285 | N | GLN | A | 174 | 34.044 | 17.871 | 16.735 | 1.00 | 31.40 | N |
| ATOM | 1286 | CA | GLN | A | 174 | 34.999 | 18.074 | 17.811 | 1.00 | 31.28 | C |
| ATOM | 1287 | C | GLN | A | 174 | 36.437 | 18.098 | 17.244 | 1.00 | 30.94 | C |
| ATOM | 1288 | O | GLN | A | 174 | 37.253 | 18.939 | 17.602 | 1.00 | 30.50 | O |
| ATOM | 1289 | CB | GLN | A | 174 | 34.808 | 16.971 | 18.861 | 1.00 | 31.20 | C |
| ATOM | 1290 | CG | GLN | A | 174 | 35.859 | 16.917 | 19.935 | 1.00 | 31.64 | C |
| ATOM | 1291 | CD | GLN | A | 174 | 35.704 | 15.717 | 20.836 | 1.00 | 31.52 | C |
| ATOM | 1292 | OE1 | GLN | A | 174 | 35.313 | 14.661 | 20.382 | 1.00 | 35.10 | O |
| ATOM | 1293 | NE2 | GLN | A | 174 | 36.007 | 15.880 | 22.121 | 1.00 | 32.92 | N |
| ATOM | 1294 | N | GLY | A | 175 | 36.732 | 17.202 | 16.317 | 1.00 | 30.54 | N |
| ATOM | 1295 | CA | GLY | A | 175 | 38.048 | 17.169 | 15.721 | 1.00 | 30.38 | C |
| ATOM | 1296 | C | GLY | A | 175 | 38.288 | 18.339 | 14.783 | 1.00 | 31.21 | C |
| ATOM | 1297 | O | GLY | A | 175 | 39.339 | 18.974 | 14.812 | 1.00 | 31.31 | O |
| ATOM | 1298 | N | LYS | A | 176 | 37.317 | 18.661 | 13.946 | 1.00 | 31.67 | N |
| ATOM | 1299 | CA | LYS | A | 176 | 37.524 | 19.767 | 13.029 | 1.00 | 32.84 | C |
| ATOM | 1300 | C | LYS | A | 176 | 37.758 | 21.127 | 13.749 | 1.00 | 32.90 | C |
| ATOM | 1301 | O | LYS | A | 176 | 38.563 | 21.906 | 13.291 | 1.00 | 32.85 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1302 | CB | LYS | A | 176 | 36.351 | 19.915 | 12.074 | 1.00 | 33.80 | C |
| ATOM | 1303 | CG | LYS | A | 176 | 36.187 | 18.832 | 11.037 | 1.00 | 35.93 | C |
| ATOM | 1304 | CD | LYS | A | 176 | 34.982 | 19.185 | 10.168 | 1.00 | 39.44 | C |
| ATOM | 1305 | CE | LYS | A | 176 | 34.055 | 18.032 | 9.961 | 1.00 | 40.94 | C |
| ATOM | 1306 | NZ | LYS | A | 176 | 32.686 | 18.495 | 9.578 | 1.00 | 45.01 | N |
| ATOM | 1307 | N | ARG | A | 177 | 37.074 | 21.398 | 14.859 | 1.00 | 32.98 | N |
| ATOM | 1308 | CA | ARG | A | 177 | 37.242 | 22.677 | 15.571 | 1.00 | 33.61 | C |
| ATOM | 1309 | C | ARG | A | 177 | 38.313 | 22.713 | 16.678 | 1.00 | 33.16 | C |
| ATOM | 1310 | O | ARG | A | 177 | 38.453 | 23.717 | 17.370 | 1.00 | 33.01 | O |
| ATOM | 1311 | CB | ARG | A | 177 | 35.920 | 23.101 | 16.220 | 1.00 | 33.86 | C |
| ATOM | 1312 | CG | ARG | A | 177 | 34.716 | 22.947 | 15.353 | 1.00 | 35.87 | C |
| ATOM | 1313 | CD | ARG | A | 177 | 34.728 | 23.721 | 14.062 | 1.00 | 37.56 | C |
| ATOM | 1314 | NE | ARG | A | 177 | 33.704 | 23.135 | 13.222 | 1.00 | 42.96 | N |
| ATOM | 1315 | CZ | ARG | A | 177 | 33.803 | 22.893 | 11.928 | 1.00 | 45.93 | C |
| ATOM | 1316 | NH1 | ARG | A | 177 | 34.897 | 23.218 | 11.247 | 1.00 | 46.65 | N |
| ATOM | 1317 | NH2 | ARG | A | 177 | 32.770 | 22.349 | 11.304 | 1.00 | 47.47 | N |
| ATOM | 1318 | N | GLY | A | 178 | 39.038 | 21.624 | 16.887 | 1.00 | 32.79 | N |
| ATOM | 1319 | CA | GLY | A | 178 | 40.068 | 21.629 | 17.907 | 1.00 | 31.78 | C |
| ATOM | 1320 | C | GLY | A | 178 | 39.511 | 21.614 | 19.313 | 1.00 | 31.64 | C |
| ATOM | 1321 | O | GLY | A | 178 | 40.251 | 21.782 | 20.292 | 1.00 | 33.25 | O |
| ATOM | 1322 | N | TRP | A | 179 | 38.223 | 21.380 | 19.468 | 1.00 | 30.56 | N |
| ATOM | 1323 | CA | TRP | A | 179 | 37.690 | 21.361 | 20.821 | 1.00 | 30.44 | C |
| ATOM | 1324 | C | TRP | A | 179 | 38.328 | 20.385 | 21.789 | 1.00 | 30.36 | C |
| ATOM | 1325 | O | TRP | A | 179 | 39.008 | 19.446 | 21.416 | 1.00 | 29.60 | O |
| ATOM | 1326 | CB | TRP | A | 179 | 36.200 | 21.115 | 20.806 | 1.00 | 30.43 | C |
| ATOM | 1327 | CG | TRP | A | 179 | 35.426 | 22.183 | 20.136 | 1.00 | 29.86 | C |
| ATOM | 1328 | CD1 | TRP | A | 179 | 35.882 | 23.409 | 19.721 | 1.00 | 27.42 | C |
| ATOM | 1329 | CD2 | TRP | A | 179 | 34.054 | 22.115 | 19.769 | 1.00 | 29.51 | C |
| ATOM | 1330 | NE1 | TRP | A | 179 | 34.870 | 24.102 | 19.104 | 1.00 | 30.05 | N |
| ATOM | 1331 | CE2 | TRP | A | 179 | 33.728 | 23.338 | 19.130 | 1.00 | 30.70 | C |
| ATOM | 1332 | CE3 | TRP | A | 179 | 33.067 | 21.145 | 19.902 | 1.00 | 27.24 | C |
| ATOM | 1333 | CZ2 | TRP | A | 179 | 32.470 | 23.602 | 18.626 | 1.00 | 27.82 | C |
| ATOM | 1334 | CZ3 | TRP | A | 179 | 31.829 | 21.397 | 19.389 | 1.00 | 28.43 | C |
| ATOM | 1335 | CH2 | TRP | A | 179 | 31.532 | 22.630 | 18.759 | 1.00 | 29.15 | C |
| ATOM | 1336 | N | GLY | A | 180 | 38.087 | 20.634 | 23.065 | 1.00 | 30.98 | N |
| ATOM | 1337 | CA | GLY | A | 180 | 38.515 | 19.723 | 24.104 | 1.00 | 30.78 | C |
| ATOM | 1338 | C | GLY | A | 180 | 37.468 | 18.637 | 24.246 | 1.00 | 31.74 | C |
| ATOM | 1339 | O | GLY | A | 180 | 36.621 | 18.448 | 23.343 | 1.00 | 31.97 | O |
| ATOM | 1340 | N | GLN | A | 181 | 37.498 | 17.941 | 25.378 | 1.00 | 32.16 | N |
| ATOM | 1341 | CA | GLN | A | 181 | 36.628 | 16.798 | 25.608 | 1.00 | 33.12 | C |
| ATOM | 1342 | C | GLN | A | 181 | 35.161 | 17.108 | 25.885 | 1.00 | 32.52 | C |
| ATOM | 1343 | O | GLN | A | 181 | 34.813 | 18.181 | 26.348 | 1.00 | 32.55 | O |
| ATOM | 1344 | CB | GLN | A | 181 | 37.161 | 15.962 | 26.773 | 1.00 | 33.24 | C |
| ATOM | 1345 | CG | GLN | A | 181 | 36.780 | 16.496 | 28.155 | 1.00 | 37.52 | C |
| ATOM | 1346 | CD | GLN | A | 181 | 37.066 | 15.488 | 29.282 | 1.00 | 42.63 | C |
| ATOM | 1347 | OE1 | GLN | A | 181 | 38.200 | 15.034 | 29.442 | 1.00 | 46.67 | O |
| ATOM | 1348 | NE2 | GLN | A | 181 | 36.037 | 15.131 | 30.043 | 1.00 | 45.13 | N |
| ATOM | 1349 | N | LEU | A | 182 | 34.310 | 16.134 | 25.588 | 1.00 | 32.12 | N |
| ATOM | 1350 | CA | LEU | A | 182 | 32.907 | 16.155 | 26.001 | 1.00 | 31.88 | C |
| ATOM | 1351 | C | LEU | A | 182 | 32.928 | 16.114 | 27.528 | 1.00 | 30.66 | C |
| ATOM | 1352 | O | LEU | A | 182 | 33.481 | 15.190 | 28.087 | 1.00 | 30.31 | O |
| ATOM | 1353 | CB | LEU | A | 182 | 32.228 | 14.880 | 25.512 | 1.00 | 31.80 | C |
| ATOM | 1354 | CG | LEU | A | 182 | 30.715 | 14.723 | 25.454 | 1.00 | 33.59 | C |
| ATOM | 1355 | CD1 | LEU | A | 182 | 30.319 | 13.250 | 25.572 | 1.00 | 32.15 | C |
| ATOM | 1356 | CD2 | LEU | A | 182 | 30.059 | 15.454 | 26.520 | 1.00 | 36.60 | C |
| ATOM | 1357 | N | THR | A | 183 | 32.373 | 17.112 | 28.207 | 1.00 | 29.62 | N |
| ATOM | 1358 | CA | THR | A | 183 | 32.383 | 17.088 | 29.657 | 1.00 | 28.62 | C |
| ATOM | 1359 | C | THR | A | 183 | 31.088 | 16.509 | 30.123 | 1.00 | 28.48 | C |
| ATOM | 1360 | O | THR | A | 183 | 31.034 | 15.991 | 31.207 | 1.00 | 28.46 | O |
| ATOM | 1361 | CB | THR | A | 183 | 32.504 | 18.509 | 30.276 | 1.00 | 28.82 | C |
| ATOM | 1362 | OG1 | THR | A | 183 | 31.441 | 19.364 | 29.795 | 1.00 | 28.93 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1363 | CG2 | THR | A | 183 | 33.764 | 19.178 | 29.846 | 1.00 | 28.28 | C |
| ATOM | 1364 | N | SER | A | 184 | 30.005 | 16.673 | 29.355 | 1.00 | 28.14 | N |
| ATOM | 1365 | CA | SER | A | 184 | 28.734 | 16.144 | 29.805 | 1.00 | 28.16 | C |
| ATOM | 1366 | C | SER | A | 184 | 27.602 | 16.374 | 28.878 | 1.00 | 28.07 | C |
| ATOM | 1367 | O | SER | A | 184 | 27.703 | 17.120 | 27.931 | 1.00 | 29.72 | O |
| ATOM | 1368 | CB | SER | A | 184 | 28.357 | 16.750 | 31.149 | 1.00 | 27.81 | C |
| ATOM | 1369 | OG | SER | A | 184 | 28.166 | 18.132 | 31.017 | 1.00 | 30.35 | O |
| ATOM | 1370 | N | ASN | A | 185 | 26.505 | 15.721 | 29.176 | 1.00 | 27.93 | N |
| ATOM | 1371 | CA | ASN | A | 185 | 25.288 | 15.850 | 28.434 | 1.00 | 28.66 | C |
| ATOM | 1372 | C | ASN | A | 185 | 24.235 | 16.086 | 29.476 | 1.00 | 28.67 | C |
| ATOM | 1373 | O | ASN | A | 185 | 23.974 | 15.226 | 30.291 | 1.00 | 27.67 | O |
| ATOM | 1374 | CB | ASN | A | 185 | 24.927 | 14.543 | 27.683 | 1.00 | 28.53 | C |
| ATOM | 1375 | CG | ASN | A | 185 | 25.914 | 14.191 | 26.589 | 1.00 | 29.19 | C |
| ATOM | 1376 | OD1 | ASN | A | 185 | 26.684 | 13.278 | 26.766 | 1.00 | 30.93 | O |
| ATOM | 1377 | ND2 | ASN | A | 185 | 25.891 | 14.910 | 25.451 | 1.00 | 29.67 | N |
| ATOM | 1378 | N | LEU | A | 186 | 23.583 | 17.221 | 29.415 | 1.00 | 29.39 | N |
| ATOM | 1379 | CA | LEU | A | 186 | 22.557 | 17.526 | 30.388 | 1.00 | 30.47 | C |
| ATOM | 1380 | C | LEU | A | 186 | 21.179 | 17.177 | 29.835 | 1.00 | 30.85 | C |
| ATOM | 1381 | O | LEU | A | 186 | 20.796 | 17.566 | 28.714 | 1.00 | 30.64 | O |
| ATOM | 1382 | CB | LEU | A | 186 | 22.617 | 18.998 | 30.730 | 1.00 | 30.48 | C |
| ATOM | 1383 | CG | LEU | A | 186 | 21.779 | 19.484 | 31.917 | 1.00 | 32.51 | C |
| ATOM | 1384 | CD1 | LEU | A | 186 | 22.330 | 18.952 | 33.238 | 1.00 | 31.55 | C |
| ATOM | 1385 | CD2 | LEU | A | 186 | 21.678 | 21.072 | 31.954 | 1.00 | 29.96 | C |
| ATOM | 1386 | N | LEU | A | 187 | 20.409 | 16.439 | 30.613 | 1.00 | 31.21 | N |
| ATOM | 1387 | CA | LEU | A | 187 | 19.042 | 16.155 | 30.188 | 1.00 | 30.60 | C |
| ATOM | 1388 | C | LEU | A | 187 | 18.162 | 17.256 | 30.787 | 1.00 | 30.79 | C |
| ATOM | 1389 | O | LEU | A | 187 | 18.257 | 17.557 | 31.991 | 1.00 | 29.69 | O |
| ATOM | 1390 | CB | LEU | A | 187 | 18.626 | 14.781 | 30.644 | 1.00 | 30.50 | C |
| ATOM | 1391 | CG | LEU | A | 187 | 17.130 | 14.465 | 30.590 | 1.00 | 32.29 | C |
| ATOM | 1392 | CD1 | LEU | A | 187 | 16.592 | 14.409 | 29.164 | 1.00 | 33.95 | C |
| ATOM | 1393 | CD2 | LEU | A | 187 | 16.864 | 13.137 | 31.270 | 1.00 | 32.62 | C |
| ATOM | 1394 | N | LEU | A | 188 | 17.390 | 17.933 | 29.939 | 1.00 | 30.75 | N |
| ATOM | 1395 | CA | LEU | A | 188 | 16.513 | 18.973 | 30.426 | 1.00 | 31.42 | C |
| ATOM | 1396 | C | LEU | A | 188 | 15.053 | 18.646 | 30.107 | 1.00 | 32.02 | C |
| ATOM | 1397 | O | LEU | A | 188 | 14.676 | 18.481 | 28.941 | 1.00 | 31.44 | O |
| ATOM | 1398 | CB | LEU | A | 188 | 16.856 | 20.323 | 29.821 | 1.00 | 31.69 | C |
| ATOM | 1399 | CG | LEU | A | 188 | 18.253 | 20.823 | 30.131 | 1.00 | 32.24 | C |
| ATOM | 1400 | CD1 | LEU | A | 188 | 19.094 | 20.883 | 28.904 | 1.00 | 32.79 | C |
| ATOM | 1401 | CD2 | LEU | A | 188 | 18.121 | 22.200 | 30.658 | 1.00 | 32.69 | C |
| ATOM | 1402 | N | ILE | A | 189 | 14.228 | 18.568 | 31.146 | 1.00 | 32.26 | N |
| ATOM | 1403 | CA | ILE | A | 189 | 12.816 | 18.305 | 30.944 | 1.00 | 32.23 | C |
| ATOM | 1404 | C | ILE | A | 189 | 12.067 | 19.386 | 31.664 | 1.00 | 32.02 | C |
| ATOM | 1405 | O | ILE | A | 189 | 12.194 | 19.520 | 32.895 | 1.00 | 31.42 | O |
| ATOM | 1406 | CB | ILE | A | 189 | 12.427 | 16.966 | 31.479 | 1.00 | 32.05 | C |
| ATOM | 1407 | CG1 | ILE | A | 189 | 13.256 | 15.894 | 30.793 | 1.00 | 33.02 | C |
| ATOM | 1408 | CG2 | ILE | A | 189 | 10.957 | 16.764 | 31.232 | 1.00 | 32.90 | C |
| ATOM | 1409 | CD1 | ILE | A | 189 | 13.006 | 14.466 | 31.277 | 1.00 | 34.20 | C |
| ATOM | 1410 | N | GLY | A | 190 | 11.279 | 20.145 | 30.898 | 1.00 | 31.94 | N |
| ATOM | 1411 | CA | GLY | A | 190 | 10.623 | 21.334 | 31.414 | 1.00 | 31.49 | C |
| ATOM | 1412 | C | GLY | A | 190 | 9.147 | 21.362 | 31.125 | 1.00 | 31.41 | C |
| ATOM | 1413 | O | GLY | A | 190 | 8.671 | 20.649 | 30.245 | 1.00 | 30.40 | O |
| ATOM | 1414 | N | MET | A | 191 | 8.433 | 22.154 | 31.914 | 1.00 | 31.55 | N |
| ATOM | 1415 | CA | MET | A | 191 | 7.027 | 22.378 | 31.697 | 1.00 | 32.41 | C |
| ATOM | 1416 | C | MET | A | 191 | 6.863 | 23.547 | 30.751 | 1.00 | 32.03 | C |
| ATOM | 1417 | O | MET | A | 191 | 7.722 | 24.435 | 30.658 | 1.00 | 32.29 | O |
| ATOM | 1418 | CB | MET | A | 191 | 6.313 | 22.672 | 33.008 | 1.00 | 33.21 | C |
| ATOM | 1419 | CG | MET | A | 191 | 6.294 | 21.499 | 33.957 | 1.00 | 35.09 | C |
| ATOM | 1420 | SD | MET | A | 191 | 5.828 | 21.953 | 35.652 | 1.00 | 39.51 | S |
| ATOM | 1421 | CE | MET | A | 191 | 4.213 | 22.512 | 35.350 | 1.00 | 39.52 | C |
| ATOM | 1422 | N | GLU | A | 192 | 5.755 | 23.539 | 30.033 | 1.00 | 31.96 | N |
| ATOM | 1423 | CA | GLU | A | 192 | 5.459 | 24.588 | 29.081 | 1.00 | 32.31 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1424 | C | GLU | A | 192 | 5.511 | 25.919 | 29.776 | 1.00 | 31.73 | C |
| ATOM | 1425 | O | GLU | A | 192 | 5.096 | 26.041 | 30.913 | 1.00 | 31.73 | O |
| ATOM | 1426 | CB | GLU | A | 192 | 4.087 | 24.375 | 28.508 | 1.00 | 33.09 | C |
| ATOM | 1427 | CG | GLU | A | 192 | 2.995 | 24.434 | 29.552 | 1.00 | 34.74 | C |
| ATOM | 1428 | CD | GLU | A | 192 | 1.679 | 23.940 | 29.019 | 1.00 | 36.73 | C |
| ATOM | 1429 | OE1 | GLU | A | 192 | 1.630 | 23.515 | 27.832 | 1.00 | 37.30 | O |
| ATOM | 1430 | OE2 | GLU | A | 192 | 0.698 | 24.001 | 29.791 | 1.00 | 38.64 | O |
| ATOM | 1431 | N | GLY | A | 193 | 6.049 | 26.926 | 29.103 | 1.00 | 31.79 | N |
| ATOM | 1432 | CA | GLY | A | 193 | 6.201 | 28.242 | 29.714 | 1.00 | 30.87 | C |
| ATOM | 1433 | C | GLY | A | 193 | 7.480 | 28.432 | 30.521 | 1.00 | 30.28 | C |
| ATOM | 1434 | O | GLY | A | 193 | 7.777 | 29.534 | 30.901 | 1.00 | 30.29 | O |
| ATOM | 1435 | N | ASN | A | 194 | 8.223 | 27.375 | 30.825 | 1.00 | 29.85 | N |
| ATOM | 1436 | CA | ASN | A | 194 | 9.460 | 27.536 | 31.604 | 1.00 | 29.38 | C |
| ATOM | 1437 | C | ASN | A | 194 | 10.473 | 28.371 | 30.840 | 1.00 | 28.61 | C |
| ATOM | 1438 | O | ASN | A | 194 | 10.606 | 28.216 | 29.615 | 1.00 | 28.58 | O |
| ATOM | 1439 | CB | ASN | A | 194 | 10.136 | 26.186 | 31.866 | 1.00 | 29.15 | C |
| ATOM | 1440 | CG | ASN | A | 194 | 9.565 | 25.445 | 33.049 | 1.00 | 29.50 | C |
| ATOM | 1441 | OD1 | ASN | A | 194 | 8.632 | 25.896 | 33.714 | 1.00 | 32.61 | O |
| ATOM | 1442 | ND2 | ASN | A | 194 | 10.146 | 24.305 | 33.334 | 1.00 | 28.53 | N |
| ATOM | 1443 | N | VAL | A | 195 | 11.221 | 29.194 | 31.561 | 1.00 | 27.70 | N |
| ATOM | 1444 | CA | VAL | A | 195 | 12.272 | 29.998 | 30.962 | 1.00 | 27.80 | C |
| ATOM | 1445 | C | VAL | A | 195 | 13.586 | 29.858 | 31.701 | 1.00 | 27.07 | C |
| ATOM | 1446 | O | VAL | A | 195 | 13.636 | 29.898 | 32.939 | 1.00 | 27.43 | O |
| ATOM | 1447 | CB | VAL | A | 195 | 11.904 | 31.520 | 31.018 | 1.00 | 28.18 | C |
| ATOM | 1448 | CG1 | VAL | A | 195 | 13.056 | 32.371 | 30.560 | 1.00 | 26.78 | C |
| ATOM | 1449 | CG2 | VAL | A | 195 | 10.662 | 31.789 | 30.187 | 1.00 | 29.06 | C |
| ATOM | 1450 | N | THR | A | 196 | 14.659 | 29.712 | 30.953 | 1.00 | 26.48 | N |
| ATOM | 1451 | CA | THR | A | 196 | 15.994 | 29.811 | 31.530 | 1.00 | 26.08 | C |
| ATOM | 1452 | C | THR | A | 196 | 16.462 | 31.184 | 31.084 | 1.00 | 27.03 | C |
| ATOM | 1453 | O | THR | A | 196 | 16.614 | 31.425 | 29.876 | 1.00 | 26.51 | O |
| ATOM | 1454 | CB | THR | A | 196 | 16.915 | 28.811 | 30.934 | 1.00 | 25.96 | C |
| ATOM | 1455 | OG1 | THR | A | 196 | 16.525 | 27.478 | 31.309 | 1.00 | 26.20 | O |
| ATOM | 1456 | CG2 | THR | A | 196 | 18.340 | 29.012 | 31.457 | 1.00 | 23.99 | C |
| ATOM | 1457 | N | PRO | A | 197 | 16.647 | 32.090 | 32.036 | 1.00 | 27.21 | N |
| ATOM | 1458 | CA | PRO | A | 197 | 17.053 | 33.451 | 31.725 | 1.00 | 27.46 | C |
| ATOM | 1459 | C | PRO | A | 197 | 18.432 | 33.512 | 31.113 | 1.00 | 27.48 | C |
| ATOM | 1460 | O | PRO | A | 197 | 19.248 | 32.588 | 31.293 | 1.00 | 27.52 | O |
| ATOM | 1461 | CB | PRO | A | 197 | 17.007 | 34.166 | 33.075 | 1.00 | 27.56 | C |
| ATOM | 1462 | CG | PRO | A | 197 | 16.226 | 33.344 | 33.924 | 1.00 | 28.15 | C |
| ATOM | 1463 | CD | PRO | A | 197 | 16.384 | 31.914 | 33.470 | 1.00 | 27.92 | C |
| ATOM | 1464 | N | ALA | A | 198 | 18.668 | 34.616 | 30.413 | 1.00 | 26.77 | N |
| ATOM | 1465 | CA | ALA | A | 198 | 19.877 | 34.830 | 29.647 | 1.00 | 26.92 | C |
| ATOM | 1466 | C | ALA | A | 198 | 21.172 | 34.681 | 30.438 | 1.00 | 27.14 | C |
| ATOM | 1467 | O | ALA | A | 198 | 21.354 | 35.278 | 31.520 | 1.00 | 25.53 | O |
| ATOM | 1468 | CB | ALA | A | 198 | 19.828 | 36.235 | 29.021 | 1.00 | 27.07 | C |
| ATOM | 1469 | N | HIS | A | 199 | 22.091 | 33.929 | 29.839 | 1.00 | 27.28 | N |
| ATOM | 1470 | CA | HIS | A | 199 | 23.399 | 33.673 | 30.424 | 1.00 | 27.81 | C |
| ATOM | 1471 | C | HIS | A | 199 | 24.319 | 33.208 | 29.333 | 1.00 | 28.09 | C |
| ATOM | 1472 | O | HIS | A | 199 | 23.857 | 32.933 | 28.197 | 1.00 | 28.34 | O |
| ATOM | 1473 | CB | HIS | A | 199 | 23.323 | 32.549 | 31.461 | 1.00 | 27.10 | C |
| ATOM | 1474 | CG | HIS | A | 199 | 22.963 | 31.221 | 30.864 | 1.00 | 29.70 | C |
| ATOM | 1475 | ND1 | HIS | A | 199 | 21.668 | 30.891 | 30.525 | 1.00 | 30.01 | N |
| ATOM | 1476 | CD2 | HIS | A | 199 | 23.728 | 30.180 | 30.463 | 1.00 | 29.60 | C |
| ATOM | 1477 | CE1 | HIS | A | 199 | 21.647 | 29.684 | 29.993 | 1.00 | 29.66 | C |
| ATOM | 1478 | NE2 | HIS | A | 199 | 22.881 | 29.236 | 29.926 | 1.00 | 30.43 | N |
| ATOM | 1479 | N | TYR | A | 200 | 25.612 | 33.104 | 29.671 | 1.00 | 28.30 | N |
| ATOM | 1480 | CA | TYR | A | 200 | 26.607 | 32.518 | 28.769 | 1.00 | 28.15 | C |
| ATOM | 1481 | C | TYR | A | 200 | 27.298 | 31.351 | 29.482 | 1.00 | 27.91 | C |
| ATOM | 1482 | O | TYR | A | 200 | 27.335 | 31.333 | 30.690 | 1.00 | 27.87 | O |
| ATOM | 1483 | CB | TYR | A | 200 | 27.585 | 33.534 | 28.217 | 1.00 | 28.02 | C |
| ATOM | 1484 | CG | TYR | A | 200 | 28.540 | 34.142 | 29.226 | 1.00 | 29.58 | C |

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ATOM   1485  CD1 TYR A 200      29.784  33.571  29.462  1.00 28.14           C
ATOM   1486  CD2 TYR A 200      28.231  35.342  29.871  1.00 29.32           C
ATOM   1487  CE1 TYR A 200      30.660  34.128  30.367  1.00 30.20           C
ATOM   1488  CE2 TYR A 200      29.107  35.919  30.777  1.00 29.61           C
ATOM   1489  CZ  TYR A 200      30.319  35.315  31.031  1.00 29.78           C
ATOM   1490  OH  TYR A 200      31.180  35.864  31.940  1.00 24.43           O
ATOM   1491  N   ASP A 201      27.797  30.363  28.727  1.00 27.73           N
ATOM   1492  CA  ASP A 201      28.461  29.180  29.302  1.00 27.65           C
ATOM   1493  C   ASP A 201      29.873  29.220  28.799  1.00 27.87           C
ATOM   1494  O   ASP A 201      30.080  29.765  27.768  1.00 27.68           O
ATOM   1495  CB  ASP A 201      27.775  27.884  28.855  1.00 26.32           C
ATOM   1496  CG  ASP A 201      26.356  27.768  29.363  1.00 25.12           C
ATOM   1497  OD1 ASP A 201      26.156  27.722  30.605  1.00 23.49           O
ATOM   1498  OD2 ASP A 201      25.360  27.687  28.589  1.00 27.18           O
ATOM   1499  N   GLU A 202      30.843  28.682  29.520  1.00 29.28           N
ATOM   1500  CA  GLU A 202      32.228  28.672  29.013  1.00 31.18           C
ATOM   1501  C   GLU A 202      32.571  27.435  28.190  1.00 31.54           C
ATOM   1502  O   GLU A 202      33.734  27.060  28.139  1.00 33.48           O
ATOM   1503  CB  GLU A 202      33.250  28.741  30.155  1.00 30.78           C
ATOM   1504  CG  GLU A 202      33.122  29.981  31.003  1.00 33.61           C
ATOM   1505  CD  GLU A 202      34.194  30.081  32.062  1.00 35.96           C
ATOM   1506  OE1 GLU A 202      34.036  29.531  33.166  1.00 41.25           O
ATOM   1507  OE2 GLU A 202      35.199  30.718  31.788  1.00 39.13           O
ATOM   1508  N   GLN A 203      31.582  26.747  27.641  1.00 31.19           N
ATOM   1509  CA  GLN A 203      31.844  25.589  26.833  1.00 30.78           C
ATOM   1510  C   GLN A 203      31.078  25.743  25.556  1.00 29.96           C
ATOM   1511  O   GLN A 203      30.213  26.581  25.462  1.00 30.22           O
ATOM   1512  CB  GLN A 203      31.427  24.315  27.546  1.00 31.32           C
ATOM   1513  CG  GLN A 203      32.364  23.971  28.725  1.00 34.97           C
ATOM   1514  CD  GLN A 203      32.204  22.548  29.288  1.00 35.23           C
ATOM   1515  OE1 GLN A 203      32.161  21.559  28.551  1.00 36.82           O
ATOM   1516  NE2 GLN A 203      32.160  22.456  30.600  1.00 35.56           N
ATOM   1517  N   GLN A 204      31.461  24.961  24.555  1.00 29.46           N
ATOM   1518  CA  GLN A 204      30.791  24.911  23.292  1.00 28.65           C
ATOM   1519  C   GLN A 204      29.641  23.941  23.494  1.00 28.27           C
ATOM   1520  O   GLN A 204      29.797  22.941  24.194  1.00 27.65           O
ATOM   1521  CB  GLN A 204      31.717  24.381  22.214  1.00 29.02           C
ATOM   1522  CG  GLN A 204      33.006  25.154  22.028  1.00 28.50           C
ATOM   1523  CD  GLN A 204      32.818  26.366  21.150  1.00 27.16           C
ATOM   1524  OE1 GLN A 204      31.690  26.742  20.846  1.00 22.90           O
ATOM   1525  NE2 GLN A 204      33.921  26.952  20.714  1.00 23.20           N
ATOM   1526  N   ASN A 205      28.497  24.219  22.864  1.00 27.36           N
ATOM   1527  CA  ASN A 205      27.302  23.424  23.058  1.00 27.13           C
ATOM   1528  C   ASN A 205      26.552  23.052  21.777  1.00 27.39           C
ATOM   1529  O   ASN A 205      26.151  23.930  20.999  1.00 27.36           O
ATOM   1530  CB  ASN A 205      26.378  24.229  23.967  1.00 26.95           C
ATOM   1531  CG  ASN A 205      25.083  23.525  24.327  1.00 27.30           C
ATOM   1532  OD1 ASN A 205      24.726  22.453  23.818  1.00 27.11           O
ATOM   1533  ND2 ASN A 205      24.319  24.190  25.171  1.00 24.64           N
ATOM   1534  N   PHE A 206      26.383  21.749  21.542  1.00 26.46           N
ATOM   1535  CA  PHE A 206      25.417  21.334  20.554  1.00 25.88           C
ATOM   1536  C   PHE A 206      24.181  20.946  21.373  1.00 25.65           C
ATOM   1537  O   PHE A 206      24.230  19.988  22.178  1.00 25.16           O
ATOM   1538  CB  PHE A 206      25.909  20.170  19.717  1.00 26.28           C
ATOM   1539  CG  PHE A 206      26.837  20.566  18.636  1.00 24.81           C
ATOM   1540  CD1 PHE A 206      26.416  21.374  17.633  1.00 26.27           C
ATOM   1541  CD2 PHE A 206      28.122  20.098  18.616  1.00 25.53           C
ATOM   1542  CE1 PHE A 206      27.248  21.736  16.634  1.00 27.05           C
ATOM   1543  CE2 PHE A 206      28.991  20.469  17.617  1.00 26.80           C
ATOM   1544  CZ  PHE A 206      28.549  21.274  16.619  1.00 28.34           C
ATOM   1545  N   PHE A 207      23.084  21.648  21.086  1.00 25.08           N
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1546 | CA | PHE | A | 207 | 21.809 | 21.625 | 21.827 | 1.00 | 25.52 | C |
| ATOM | 1547 | C | PHE | A | 207 | 20.775 | 20.885 | 21.011 | 1.00 | 25.55 | C |
| ATOM | 1548 | O | PHE | A | 207 | 20.261 | 21.410 | 20.058 | 1.00 | 25.61 | O |
| ATOM | 1549 | CB | PHE | A | 207 | 21.408 | 23.107 | 22.074 | 1.00 | 25.37 | C |
| ATOM | 1550 | CG | PHE | A | 207 | 20.146 | 23.346 | 22.872 | 1.00 | 23.70 | C |
| ATOM | 1551 | CD1 | PHE | A | 207 | 18.938 | 23.547 | 22.234 | 1.00 | 24.08 | C |
| ATOM | 1552 | CD2 | PHE | A | 207 | 20.199 | 23.551 | 24.220 | 1.00 | 25.24 | C |
| ATOM | 1553 | CE1 | PHE | A | 207 | 17.800 | 23.864 | 22.927 | 1.00 | 24.50 | C |
| ATOM | 1554 | CE2 | PHE | A | 207 | 19.035 | 23.883 | 24.959 | 1.00 | 26.04 | C |
| ATOM | 1555 | CZ | PHE | A | 207 | 17.836 | 24.021 | 24.298 | 1.00 | 26.68 | C |
| ATOM | 1556 | N | ALA | A | 208 | 20.490 | 19.657 | 21.422 | 1.00 | 26.60 | N |
| ATOM | 1557 | CA | ALA | A | 208 | 19.667 | 18.710 | 20.689 | 1.00 | 26.45 | C |
| ATOM | 1558 | C | ALA | A | 208 | 18.231 | 18.594 | 21.210 | 1.00 | 27.10 | C |
| ATOM | 1559 | O | ALA | A | 208 | 17.966 | 17.987 | 22.273 | 1.00 | 26.47 | O |
| ATOM | 1560 | CB | ALA | A | 208 | 20.303 | 17.363 | 20.766 | 1.00 | 25.67 | C |
| ATOM | 1561 | N | GLN | A | 209 | 17.306 | 19.121 | 20.419 | 1.00 | 27.02 | N |
| ATOM | 1562 | CA | GLN | A | 209 | 15.918 | 19.125 | 20.833 | 1.00 | 27.37 | C |
| ATOM | 1563 | C | GLN | A | 209 | 15.276 | 17.781 | 20.519 | 1.00 | 27.55 | C |
| ATOM | 1564 | O | GLN | A | 209 | 15.489 | 17.190 | 19.427 | 1.00 | 26.51 | O |
| ATOM | 1565 | CB | GLN | A | 209 | 15.195 | 20.301 | 20.179 | 1.00 | 27.15 | C |
| ATOM | 1566 | CG | GLN | A | 209 | 13.806 | 20.508 | 20.662 | 1.00 | 27.77 | C |
| ATOM | 1567 | CD | GLN | A | 209 | 13.740 | 20.959 | 22.126 | 1.00 | 29.40 | C |
| ATOM | 1568 | OE1 | GLN | A | 209 | 14.773 | 21.166 | 22.774 | 1.00 | 27.27 | O |
| ATOM | 1569 | NE2 | GLN | A | 209 | 12.517 | 21.118 | 22.636 | 1.00 | 27.15 | N |
| ATOM | 1570 | N | ILE | A | 210 | 14.461 | 17.327 | 21.473 | 1.00 | 28.32 | N |
| ATOM | 1571 | CA | ILE | A | 210 | 13.897 | 15.998 | 21.429 | 1.00 | 29.37 | C |
| ATOM | 1572 | C | ILE | A | 210 | 12.403 | 15.966 | 21.435 | 1.00 | 30.37 | C |
| ATOM | 1573 | O | ILE | A | 210 | 11.849 | 15.275 | 20.619 | 1.00 | 31.58 | O |
| ATOM | 1574 | CB | ILE | A | 210 | 14.413 | 15.204 | 22.605 | 1.00 | 29.80 | C |
| ATOM | 1575 | CG1 | ILE | A | 210 | 15.830 | 14.734 | 22.302 | 1.00 | 30.27 | C |
| ATOM | 1576 | CG2 | ILE | A | 210 | 13.525 | 14.005 | 22.864 | 1.00 | 30.25 | C |
| ATOM | 1577 | CD1 | ILE | A | 210 | 16.624 | 14.421 | 23.516 | 1.00 | 32.28 | C |
| ATOM | 1578 | N | LYS | A | 211 | 11.757 | 16.664 | 22.374 | 1.00 | 31.18 | N |
| ATOM | 1579 | CA | LYS | A | 211 | 10.300 | 16.723 | 22.438 | 1.00 | 31.16 | C |
| ATOM | 1580 | C | LYS | A | 211 | 9.887 | 18.137 | 22.706 | 1.00 | 31.19 | C |
| ATOM | 1581 | O | LYS | A | 211 | 10.495 | 18.800 | 23.523 | 1.00 | 31.21 | O |
| ATOM | 1582 | CB | LYS | A | 211 | 9.767 | 15.891 | 23.591 | 1.00 | 32.00 | C |
| ATOM | 1583 | CG | LYS | A | 211 | 8.240 | 15.758 | 23.629 | 1.00 | 32.36 | C |
| ATOM | 1584 | CD | LYS | A | 211 | 7.787 | 15.177 | 24.970 | 1.00 | 33.23 | C |
| ATOM | 1585 | CE | LYS | A | 211 | 6.497 | 14.368 | 24.883 | 1.00 | 35.14 | C |
| ATOM | 1586 | NZ | LYS | A | 211 | 5.506 | 14.755 | 23.835 | 1.00 | 35.43 | N |
| ATOM | 1587 | N | GLY | A | 212 | 8.844 | 18.592 | 22.018 | 1.00 | 31.20 | N |
| ATOM | 1588 | CA | GLY | A | 212 | 8.337 | 19.934 | 22.174 | 1.00 | 30.96 | C |
| ATOM | 1589 | C | GLY | A | 212 | 9.209 | 20.975 | 21.495 | 1.00 | 31.42 | C |
| ATOM | 1590 | O | GLY | A | 212 | 10.167 | 20.670 | 20.771 | 1.00 | 31.06 | O |
| ATOM | 1591 | N | TYR | A | 213 | 8.857 | 22.224 | 21.734 | 1.00 | 31.43 | N |
| ATOM | 1592 | CA | TYR | A | 213 | 9.507 | 23.319 | 21.057 | 1.00 | 31.80 | C |
| ATOM | 1593 | C | TYR | A | 213 | 10.046 | 24.332 | 22.043 | 1.00 | 31.00 | C |
| ATOM | 1594 | O | TYR | A | 213 | 9.411 | 24.649 | 23.038 | 1.00 | 29.31 | O |
| ATOM | 1595 | CB | TYR | A | 213 | 8.502 | 23.959 | 20.127 | 1.00 | 32.64 | C |
| ATOM | 1596 | CG | TYR | A | 213 | 8.103 | 23.039 | 19.015 | 1.00 | 35.60 | C |
| ATOM | 1597 | CD1 | TYR | A | 213 | 7.089 | 22.071 | 19.174 | 1.00 | 38.37 | C |
| ATOM | 1598 | CD2 | TYR | A | 213 | 8.758 | 23.110 | 17.813 | 1.00 | 37.73 | C |
| ATOM | 1599 | CE1 | TYR | A | 213 | 6.765 | 21.223 | 18.137 | 1.00 | 39.37 | C |
| ATOM | 1600 | CE2 | TYR | A | 213 | 8.443 | 22.292 | 16.792 | 1.00 | 39.75 | C |
| ATOM | 1601 | CZ | TYR | A | 213 | 7.460 | 21.364 | 16.924 | 1.00 | 41.66 | C |
| ATOM | 1602 | OH | TYR | A | 213 | 7.232 | 20.603 | 15.782 | 1.00 | 46.53 | O |
| ATOM | 1603 | N | LYS | A | 214 | 11.260 | 24.787 | 21.777 | 1.00 | 30.99 | N |
| ATOM | 1604 | CA | LYS | A | 214 | 11.886 | 25.804 | 22.594 | 1.00 | 31.15 | C |
| ATOM | 1605 | C | LYS | A | 214 | 12.305 | 26.993 | 21.762 | 1.00 | 31.00 | C |
| ATOM | 1606 | O | LYS | A | 214 | 12.914 | 26.838 | 20.695 | 1.00 | 31.84 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1607 | CB | LYS | A | 214 | 13.112 | 25.244 | 23.311 | 1.00 | 31.08 | C |
| ATOM | 1608 | CG | LYS | A | 214 | 12.806 | 24.432 | 24.557 | 1.00 | 30.96 | C |
| ATOM | 1609 | CD | LYS | A | 214 | 14.106 | 23.949 | 25.159 | 1.00 | 30.84 | C |
| ATOM | 1610 | CE | LYS | A | 214 | 13.982 | 23.555 | 26.584 | 1.00 | 29.59 | C |
| ATOM | 1611 | NZ | LYS | A | 214 | 15.278 | 23.118 | 27.162 | 1.00 | 28.16 | N |
| ATOM | 1612 | N | ARG | A | 215 | 11.992 | 28.193 | 22.241 | 1.00 | 30.59 | N |
| ATOM | 1613 | CA | ARG | A | 215 | 12.445 | 29.385 | 21.549 | 1.00 | 29.98 | C |
| ATOM | 1614 | C | ARG | A | 215 | 13.764 | 29.790 | 22.154 | 1.00 | 29.65 | C |
| ATOM | 1615 | O | ARG | A | 215 | 13.850 | 29.982 | 23.349 | 1.00 | 29.61 | O |
| ATOM | 1616 | CB | ARG | A | 215 | 11.431 | 30.502 | 21.690 | 1.00 | 30.08 | C |
| ATOM | 1617 | CG | ARG | A | 215 | 11.835 | 31.810 | 21.004 | 1.00 | 29.82 | C |
| ATOM | 1618 | CD | ARG | A | 215 | 11.221 | 32.960 | 21.731 | 1.00 | 32.78 | C |
| ATOM | 1619 | NE | ARG | A | 215 | 11.211 | 34.189 | 20.975 | 1.00 | 33.81 | N |
| ATOM | 1620 | CZ | ARG | A | 215 | 10.540 | 35.259 | 21.336 | 1.00 | 35.12 | C |
| ATOM | 1621 | NH1 | ARG | A | 215 | 9.828 | 35.262 | 22.441 | 1.00 | 35.28 | N |
| ATOM | 1622 | NH2 | ARG | A | 215 | 10.586 | 36.338 | 20.581 | 1.00 | 39.28 | N |
| ATOM | 1623 | N | CYS | A | 216 | 14.791 | 29.909 | 21.327 | 1.00 | 29.86 | N |
| ATOM | 1624 | CA | CYS | A | 216 | 16.129 | 30.237 | 21.797 | 1.00 | 29.64 | C |
| ATOM | 1625 | C | CYS | A | 216 | 16.533 | 31.603 | 21.274 | 1.00 | 30.06 | C |
| ATOM | 1626 | O | CYS | A | 216 | 16.516 | 31.807 | 20.092 | 1.00 | 31.32 | O |
| ATOM | 1627 | CB | CYS | A | 216 | 17.113 | 29.183 | 21.275 | 1.00 | 29.78 | C |
| ATOM | 1628 | SG | CYS | A | 216 | 16.658 | 27.438 | 21.641 | 1.00 | 30.35 | S |
| ATOM | 1629 | N | ILE | A | 217 | 16.849 | 32.556 | 22.149 | 1.00 | 30.28 | N |
| ATOM | 1630 | CA | ILE | A | 217 | 17.303 | 33.876 | 21.744 | 1.00 | 29.78 | C |
| ATOM | 1631 | C | ILE | A | 217 | 18.758 | 34.017 | 22.203 | 1.00 | 29.42 | C |
| ATOM | 1632 | O | ILE | A | 217 | 19.050 | 33.852 | 23.385 | 1.00 | 28.77 | O |
| ATOM | 1633 | CB | ILE | A | 217 | 16.427 | 34.969 | 22.391 | 1.00 | 30.51 | C |
| ATOM | 1634 | CG1 | ILE | A | 217 | 14.934 | 34.705 | 22.111 | 1.00 | 31.29 | C |
| ATOM | 1635 | CG2 | ILE | A | 217 | 16.785 | 36.313 | 21.843 | 1.00 | 30.11 | C |
| ATOM | 1636 | CD1 | ILE | A | 217 | 14.009 | 35.655 | 22.847 | 1.00 | 33.08 | C |
| ATOM | 1637 | N | LEU | A | 218 | 19.647 | 34.326 | 21.257 | 1.00 | 28.60 | N |
| ATOM | 1638 | CA | LEU | A | 218 | 21.059 | 34.392 | 21.501 | 1.00 | 28.59 | C |
| ATOM | 1639 | C | LEU | A | 218 | 21.606 | 35.781 | 21.257 | 1.00 | 28.74 | C |
| ATOM | 1640 | O | LEU | A | 218 | 21.102 | 36.522 | 20.412 | 1.00 | 29.64 | O |
| ATOM | 1641 | CB | LEU | A | 218 | 21.788 | 33.422 | 20.574 | 1.00 | 28.52 | C |
| ATOM | 1642 | CG | LEU | A | 218 | 21.927 | 31.980 | 21.028 | 1.00 | 28.46 | C |
| ATOM | 1643 | CD1 | LEU | A | 218 | 20.569 | 31.318 | 21.233 | 1.00 | 28.95 | C |
| ATOM | 1644 | CD2 | LEU | A | 218 | 22.707 | 31.196 | 20.026 | 1.00 | 27.94 | C |
| ATOM | 1645 | N | PHE | A | 219 | 22.659 | 36.145 | 21.986 | 1.00 | 28.61 | N |
| ATOM | 1646 | CA | PHE | A | 219 | 23.309 | 37.458 | 21.774 | 1.00 | 28.07 | C |
| ATOM | 1647 | C | PHE | A | 219 | 24.811 | 37.221 | 21.710 | 1.00 | 28.25 | C |
| ATOM | 1648 | O | PHE | A | 219 | 25.352 | 36.468 | 22.517 | 1.00 | 28.82 | O |
| ATOM | 1649 | CB | PHE | A | 219 | 22.987 | 38.415 | 22.908 | 1.00 | 26.73 | C |
| ATOM | 1650 | CG | PHE | A | 219 | 21.522 | 38.553 | 23.199 | 1.00 | 27.28 | C |
| ATOM | 1651 | CD1 | PHE | A | 219 | 20.874 | 37.658 | 24.029 | 1.00 | 25.73 | C |
| ATOM | 1652 | CD2 | PHE | A | 219 | 20.782 | 39.598 | 22.648 | 1.00 | 28.57 | C |
| ATOM | 1653 | CE1 | PHE | A | 219 | 19.536 | 37.811 | 24.311 | 1.00 | 26.59 | C |
| ATOM | 1654 | CE2 | PHE | A | 219 | 19.443 | 39.722 | 22.898 | 1.00 | 27.78 | C |
| ATOM | 1655 | CZ | PHE | A | 219 | 18.816 | 38.828 | 23.725 | 1.00 | 28.22 | C |
| ATOM | 1656 | N | PRO | A | 220 | 25.501 | 37.840 | 20.776 | 1.00 | 28.30 | N |
| ATOM | 1657 | CA | PRO | A | 220 | 26.946 | 37.641 | 20.675 | 1.00 | 28.76 | C |
| ATOM | 1658 | C | PRO | A | 220 | 27.688 | 38.195 | 21.881 | 1.00 | 29.07 | C |
| ATOM | 1659 | O | PRO | A | 220 | 27.172 | 39.019 | 22.661 | 1.00 | 29.11 | O |
| ATOM | 1660 | CB | PRO | A | 220 | 27.336 | 38.413 | 19.426 | 1.00 | 28.79 | C |
| ATOM | 1661 | CG | PRO | A | 220 | 26.016 | 38.847 | 18.795 | 1.00 | 29.65 | C |
| ATOM | 1662 | CD | PRO | A | 220 | 24.987 | 38.794 | 19.790 | 1.00 | 28.85 | C |
| ATOM | 1663 | N | PRO | A | 221 | 28.914 | 37.727 | 22.057 | 1.00 | 29.09 | N |
| ATOM | 1664 | CA | PRO | A | 221 | 29.725 | 38.147 | 23.188 | 1.00 | 28.85 | C |
| ATOM | 1665 | C | PRO | A | 221 | 29.979 | 39.656 | 23.199 | 1.00 | 28.60 | C |
| ATOM | 1666 | O | PRO | A | 221 | 30.223 | 40.182 | 24.270 | 1.00 | 26.85 | O |
| ATOM | 1667 | CB | PRO | A | 221 | 31.018 | 37.412 | 22.975 | 1.00 | 29.01 | C |

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ATOM   1668  CG  PRO A 221      30.665  36.286  22.114  1.00 30.46           C
ATOM   1669  CD  PRO A 221      29.580  36.722  21.232  1.00 29.52           C
ATOM   1670  N   ASP A 222      29.853  40.335  22.062  1.00 28.17           N
ATOM   1671  CA  ASP A 222      30.155  41.763  22.044  1.00 28.79           C
ATOM   1672  C   ASP A 222      28.976  42.554  22.533  1.00 28.84           C
ATOM   1673  O   ASP A 222      28.948  43.767  22.432  1.00 30.46           O
ATOM   1674  CB  ASP A 222      30.631  42.287  20.693  1.00 27.27           C
ATOM   1675  CG  ASP A 222      29.541  42.288  19.655  1.00 30.76           C
ATOM   1676  OD1 ASP A 222      28.368  41.926  19.920  1.00 30.56           O
ATOM   1677  OD2 ASP A 222      29.785  42.609  18.495  1.00 39.36           O
ATOM   1678  N   GLN A 223      28.000  41.885  23.083  1.00 29.33           N
ATOM   1679  CA  GLN A 223      26.902  42.614  23.676  1.00 29.61           C
ATOM   1680  C   GLN A 223      27.012  42.533  25.194  1.00 28.97           C
ATOM   1681  O   GLN A 223      26.065  42.825  25.919  1.00 29.82           O
ATOM   1682  CB  GLN A 223      25.575  42.131  23.110  1.00 30.22           C
ATOM   1683  CG  GLN A 223      25.244  42.854  21.762  1.00 33.01           C
ATOM   1684  CD  GLN A 223      23.866  42.562  21.241  1.00 37.71           C
ATOM   1685  OE1 GLN A 223      22.899  42.573  22.005  1.00 43.11           O
ATOM   1686  NE2 GLN A 223      23.760  42.285  19.943  1.00 38.91           N
ATOM   1687  N   PHE A 224      28.181  42.148  25.672  1.00 27.69           N
ATOM   1688  CA  PHE A 224      28.452  42.168  27.115  1.00 28.30           C
ATOM   1689  C   PHE A 224      27.932  43.497  27.771  1.00 29.27           C
ATOM   1690  O   PHE A 224      27.248  43.448  28.786  1.00 29.24           O
ATOM   1691  CB  PHE A 224      29.968  42.025  27.373  1.00 26.64           C
ATOM   1692  CG  PHE A 224      30.338  41.881  28.810  1.00 27.05           C
ATOM   1693  CD1 PHE A 224      30.526  42.992  29.619  1.00 26.91           C
ATOM   1694  CD2 PHE A 224      30.560  40.649  29.365  1.00 25.77           C
ATOM   1695  CE1 PHE A 224      30.878  42.864  30.930  1.00 24.95           C
ATOM   1696  CE2 PHE A 224      30.928  40.522  30.675  1.00 25.92           C
ATOM   1697  CZ  PHE A 224      31.056  41.641  31.467  1.00 27.45           C
ATOM   1698  N   GLU A 225      28.253  44.658  27.177  1.00 30.23           N
ATOM   1699  CA  GLU A 225      27.873  45.951  27.753  1.00 31.35           C
ATOM   1700  C   GLU A 225      26.362  46.120  27.909  1.00 30.48           C
ATOM   1701  O   GLU A 225      25.925  46.920  28.738  1.00 28.49           O
ATOM   1702  CB  GLU A 225      28.401  47.130  26.927  1.00 32.35           C
ATOM   1703  CG  GLU A 225      29.894  47.356  27.083  1.00 37.72           C
ATOM   1704  CD  GLU A 225      30.327  48.801  27.406  1.00 45.22           C
ATOM   1705  OE1 GLU A 225      29.848  49.472  28.389  1.00 44.87           O
ATOM   1706  OE2 GLU A 225      31.230  49.248  26.665  1.00 54.04           O
ATOM   1707  N   CYS A 226      25.579  45.375  27.116  1.00 29.44           N
ATOM   1708  CA  CYS A 226      24.132  45.532  27.155  1.00 28.60           C
ATOM   1709  C   CYS A 226      23.429  44.524  28.056  1.00 28.86           C
ATOM   1710  O   CYS A 226      22.236  44.716  28.352  1.00 27.16           O
ATOM   1711  CB  CYS A 226      23.541  45.373  25.767  1.00 29.07           C
ATOM   1712  SG  CYS A 226      24.193  46.391  24.441  1.00 29.66           S
ATOM   1713  N   LEU A 227      24.133  43.455  28.483  1.00 28.37           N
ATOM   1714  CA  LEU A 227      23.469  42.390  29.242  1.00 28.53           C
ATOM   1715  C   LEU A 227      23.760  42.287  30.737  1.00 27.80           C
ATOM   1716  O   LEU A 227      23.117  41.540  31.465  1.00 26.98           O
ATOM   1717  CB  LEU A 227      23.701  41.062  28.531  1.00 28.86           C
ATOM   1718  CG  LEU A 227      22.853  41.135  27.246  1.00 30.66           C
ATOM   1719  CD1 LEU A 227      23.335  40.152  26.186  1.00 32.05           C
ATOM   1720  CD2 LEU A 227      21.389  40.812  27.590  1.00 30.73           C
ATOM   1721  N   TYR A 228      24.760  43.016  31.170  1.00 28.05           N
ATOM   1722  CA  TYR A 228      25.034  43.219  32.596  1.00 28.59           C
ATOM   1723  C   TYR A 228      25.051  41.978  33.504  1.00 29.27           C
ATOM   1724  O   TYR A 228      24.253  41.863  34.483  1.00 29.59           O
ATOM   1725  CB  TYR A 228      24.026  44.213  33.157  1.00 28.04           C
ATOM   1726  CG  TYR A 228      24.019  45.556  32.464  1.00 28.00           C
ATOM   1727  CD1 TYR A 228      24.839  46.584  32.881  1.00 27.54           C
ATOM   1728  CD2 TYR A 228      23.177  45.799  31.389  1.00 28.83           C
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ATOM   1729  CE1 TYR A 228      24.826  47.828  32.248  1.00 27.44           C
ATOM   1730  CE2 TYR A 228      23.160  47.018  30.745  1.00 27.63           C
ATOM   1731  CZ  TYR A 228      23.964  48.040  31.186  1.00 29.01           C
ATOM   1732  OH  TYR A 228      23.924  49.260  30.536  1.00 28.98           O
ATOM   1733  N   PRO A 229      26.009  41.101  33.261  1.00 28.11           N
ATOM   1734  CA  PRO A 229      26.146  39.900  34.082  1.00 28.54           C
ATOM   1735  C   PRO A 229      26.424  40.223  35.534  1.00 27.88           C
ATOM   1736  O   PRO A 229      27.085  41.212  35.786  1.00 28.01           O
ATOM   1737  CB  PRO A 229      27.396  39.214  33.494  1.00 28.67           C
ATOM   1738  CG  PRO A 229      28.116  40.314  32.802  1.00 28.96           C
ATOM   1739  CD  PRO A 229      27.046  41.191  32.231  1.00 28.25           C
ATOM   1740  N   TYR A 230      25.981  39.372  36.453  1.00 26.80           N
ATOM   1741  CA  TYR A 230      26.296  39.542  37.840  1.00 25.91           C
ATOM   1742  C   TYR A 230      27.838  39.508  38.028  1.00 25.72           C
ATOM   1743  O   TYR A 230      28.582  39.094  37.167  1.00 25.79           O
ATOM   1744  CB  TYR A 230      25.673  38.431  38.677  1.00 25.13           C
ATOM   1745  CG  TYR A 230      24.193  38.523  38.900  1.00 24.95           C
ATOM   1746  CD1 TYR A 230      23.289  38.036  37.933  1.00 24.25           C
ATOM   1747  CD2 TYR A 230      23.675  39.063  40.090  1.00 25.16           C
ATOM   1748  CE1 TYR A 230      21.944  38.105  38.139  1.00 24.40           C
ATOM   1749  CE2 TYR A 230      22.311  39.114  40.320  1.00 23.86           C
ATOM   1750  CZ  TYR A 230      21.464  38.647  39.336  1.00 26.74           C
ATOM   1751  OH  TYR A 230      20.122  38.713  39.501  1.00 34.04           O
ATOM   1752  N   PRO A 231      28.309  39.966  39.167  1.00 25.05           N
ATOM   1753  CA  PRO A 231      29.711  39.806  39.517  1.00 24.73           C
ATOM   1754  C   PRO A 231      30.151  38.318  39.500  1.00 24.94           C
ATOM   1755  O   PRO A 231      29.359  37.410  39.817  1.00 24.30           O
ATOM   1756  CB  PRO A 231      29.760  40.353  40.957  1.00 25.28           C
ATOM   1757  CG  PRO A 231      28.613  41.331  41.016  1.00 25.28           C
ATOM   1758  CD  PRO A 231      27.535  40.687  40.198  1.00 24.73           C
ATOM   1759  N   VAL A 232      31.419  38.086  39.173  1.00 23.75           N
ATOM   1760  CA  VAL A 232      31.898  36.766  39.055  1.00 24.45           C
ATOM   1761  C   VAL A 232      31.725  35.935  40.351  1.00 24.83           C
ATOM   1762  O   VAL A 232      31.402  34.754  40.263  1.00 24.83           O
ATOM   1763  CB  VAL A 232      33.375  36.761  38.582  1.00 25.13           C
ATOM   1764  CG1 VAL A 232      33.974  35.405  38.828  1.00 23.91           C
ATOM   1765  CG2 VAL A 232      33.481  37.091  37.092  1.00 23.86           C
ATOM   1766  N   HIS A 233      31.886  36.540  41.525  1.00 25.24           N
ATOM   1767  CA  HIS A 233      31.766  35.806  42.790  1.00 26.43           C
ATOM   1768  C   HIS A 233      30.321  35.656  43.304  1.00 26.47           C
ATOM   1769  O   HIS A 233      30.052  34.986  44.289  1.00 26.08           O
ATOM   1770  CB  HIS A 233      32.617  36.475  43.855  1.00 26.65           C
ATOM   1771  CG  HIS A 233      34.078  36.428  43.564  1.00 28.51           C
ATOM   1772  ND1 HIS A 233      34.764  37.493  43.013  1.00 30.95           N
ATOM   1773  CD2 HIS A 233      34.987  35.435  43.730  1.00 29.75           C
ATOM   1774  CE1 HIS A 233      36.043  37.169  42.888  1.00 31.18           C
ATOM   1775  NE2 HIS A 233      36.201  35.919  43.302  1.00 32.10           N
ATOM   1776  N   HIS A 234      29.391  36.283  42.626  1.00 26.94           N
ATOM   1777  CA  HIS A 234      27.999  36.141  42.983  1.00 27.89           C
ATOM   1778  C   HIS A 234      27.456  34.838  42.411  1.00 27.85           C
ATOM   1779  O   HIS A 234      27.871  34.403  41.384  1.00 27.14           O
ATOM   1780  CB  HIS A 234      27.219  37.258  42.372  1.00 28.20           C
ATOM   1781  CG  HIS A 234      25.782  37.279  42.748  1.00 27.95           C
ATOM   1782  ND1 HIS A 234      24.840  36.514  42.092  1.00 30.05           N
ATOM   1783  CD2 HIS A 234      25.105  38.057  43.624  1.00 26.43           C
ATOM   1784  CE1 HIS A 234      23.644  36.789  42.588  1.00 29.87           C
ATOM   1785  NE2 HIS A 234      23.781  37.714  43.524  1.00 27.85           N
ATOM   1786  N   PRO A 235      26.561  34.197  43.130  1.00 28.44           N
ATOM   1787  CA  PRO A 235      26.018  32.929  42.678  1.00 28.87           C
ATOM   1788  C   PRO A 235      25.431  32.956  41.294  1.00 28.34           C
ATOM   1789  O   PRO A 235      25.387  31.884  40.716  1.00 28.04           O
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1790 | CB | PRO A 235 | 24.931 | 32.636 | 43.713 | 1.00 | 29.59 | C |
| ATOM | 1791 | CG | PRO A 235 | 25.473 | 33.290 | 44.975 | 1.00 | 29.10 | C |
| ATOM | 1792 | CD | PRO A 235 | 26.059 | 34.571 | 44.466 | 1.00 | 28.17 | C |
| ATOM | 1793 | N | CYS A 236 | 25.021 | 34.112 | 40.770 | 1.00 | 27.29 | N |
| ATOM | 1794 | CA | CYS A 236 | 24.447 | 34.135 | 39.455 | 1.00 | 26.15 | C |
| ATOM | 1795 | C | CYS A 236 | 25.478 | 34.602 | 38.451 | 1.00 | 25.39 | C |
| ATOM | 1796 | O | CYS A 236 | 25.140 | 35.102 | 37.361 | 1.00 | 26.21 | O |
| ATOM | 1797 | CB | CYS A 236 | 23.158 | 34.923 | 39.436 | 1.00 | 26.36 | C |
| ATOM | 1798 | SG | CYS A 236 | 21.908 | 34.207 | 40.555 | 1.00 | 29.77 | S |
| ATOM | 1799 | N | ASP A 237 | 26.746 | 34.411 | 38.803 | 1.00 | 24.07 | N |
| ATOM | 1800 | CA | ASP A 237 | 27.830 | 34.528 | 37.855 | 1.00 | 24.53 | C |
| ATOM | 1801 | C | ASP A 237 | 27.441 | 33.977 | 36.467 | 1.00 | 24.31 | C |
| ATOM | 1802 | O | ASP A 237 | 26.966 | 32.865 | 36.344 | 1.00 | 23.00 | O |
| ATOM | 1803 | CB | ASP A 237 | 29.018 | 33.769 | 38.353 | 1.00 | 24.42 | C |
| ATOM | 1804 | CG | ASP A 237 | 30.233 | 33.850 | 37.414 | 1.00 | 28.30 | C |
| ATOM | 1805 | OD1 | ASP A 237 | 30.433 | 34.877 | 36.673 | 1.00 | 29.51 | O |
| ATOM | 1806 | OD2 | ASP A 237 | 31.071 | 32.900 | 37.386 | 1.00 | 29.51 | O |
| ATOM | 1807 | N | ARG A 238 | 27.633 | 34.803 | 35.445 | 1.00 | 24.85 | N |
| ATOM | 1808 | CA | ARG A 238 | 27.388 | 34.434 | 34.041 | 1.00 | 26.59 | C |
| ATOM | 1809 | C | ARG A 238 | 25.921 | 34.663 | 33.595 | 1.00 | 25.95 | C |
| ATOM | 1810 | O | ARG A 238 | 25.647 | 34.628 | 32.426 | 1.00 | 26.55 | O |
| ATOM | 1811 | CB | ARG A 238 | 27.834 | 32.994 | 33.737 | 1.00 | 26.57 | C |
| ATOM | 1812 | CG | ARG A 238 | 29.311 | 32.758 | 33.891 | 1.00 | 27.77 | C |
| ATOM | 1813 | CD | ARG A 238 | 29.727 | 31.360 | 33.399 | 1.00 | 28.78 | C |
| ATOM | 1814 | NE | ARG A 238 | 29.142 | 30.434 | 34.337 | 1.00 | 33.68 | N |
| ATOM | 1815 | CZ | ARG A 238 | 28.046 | 29.736 | 34.140 | 1.00 | 36.98 | C |
| ATOM | 1816 | NH1 | ARG A 238 | 27.383 | 29.782 | 32.980 | 1.00 | 38.06 | N |
| ATOM | 1817 | NH2 | ARG A 238 | 27.609 | 28.987 | 35.129 | 1.00 | 37.87 | N |
| ATOM | 1818 | N | GLN A 239 | 25.012 | 34.933 | 34.516 | 1.00 | 25.97 | N |
| ATOM | 1819 | CA | GLN A 239 | 23.634 | 35.245 | 34.152 | 1.00 | 26.05 | C |
| ATOM | 1820 | C | GLN A 239 | 23.478 | 36.776 | 34.037 | 1.00 | 26.67 | C |
| ATOM | 1821 | O | GLN A 239 | 24.196 | 37.531 | 34.699 | 1.00 | 27.33 | O |
| ATOM | 1822 | CB | GLN A 239 | 22.663 | 34.724 | 35.201 | 1.00 | 25.55 | C |
| ATOM | 1823 | CG | GLN A 239 | 23.027 | 33.417 | 35.843 | 1.00 | 27.73 | C |
| ATOM | 1824 | CD | GLN A 239 | 23.246 | 32.282 | 34.859 | 1.00 | 31.42 | C |
| ATOM | 1825 | OE1 | GLN A 239 | 22.332 | 31.881 | 34.133 | 1.00 | 34.43 | O |
| ATOM | 1826 | NE2 | GLN A 239 | 24.457 | 31.761 | 34.835 | 1.00 | 31.35 | N |
| ATOM | 1827 | N | SER A 240 | 22.569 | 37.233 | 33.185 | 1.00 | 26.94 | N |
| ATOM | 1828 | CA | SER A 240 | 22.293 | 38.653 | 33.034 | 1.00 | 26.93 | C |
| ATOM | 1829 | C | SER A 240 | 21.490 | 39.118 | 34.229 | 1.00 | 26.78 | C |
| ATOM | 1830 | O | SER A 240 | 20.642 | 38.389 | 34.703 | 1.00 | 27.00 | O |
| ATOM | 1831 | CB | SER A 240 | 21.414 | 38.891 | 31.818 | 1.00 | 26.95 | C |
| ATOM | 1832 | OG | SER A 240 | 20.916 | 40.234 | 31.804 | 1.00 | 27.75 | O |
| ATOM | 1833 | N | GLN A 241 | 21.733 | 40.331 | 34.696 | 1.00 | 26.90 | N |
| ATOM | 1834 | CA | GLN A 241 | 20.963 | 40.903 | 35.816 | 1.00 | 27.25 | C |
| ATOM | 1835 | C | GLN A 241 | 19.632 | 41.520 | 35.311 | 1.00 | 27.84 | C |
| ATOM | 1836 | O | GLN A 241 | 18.763 | 41.866 | 36.104 | 1.00 | 27.28 | O |
| ATOM | 1837 | CB | GLN A 241 | 21.734 | 42.009 | 36.546 | 1.00 | 26.21 | C |
| ATOM | 1838 | CG | GLN A 241 | 22.971 | 41.636 | 37.344 | 1.00 | 26.53 | C |
| ATOM | 1839 | CD | GLN A 241 | 23.740 | 42.877 | 37.817 | 1.00 | 26.65 | C |
| ATOM | 1840 | OE1 | GLN A 241 | 23.436 | 43.425 | 38.859 | 1.00 | 31.02 | O |
| ATOM | 1841 | NE2 | GLN A 241 | 24.714 | 43.318 | 37.048 | 1.00 | 28.00 | N |
| ATOM | 1842 | N | VAL A 242 | 19.464 | 41.657 | 34.004 | 1.00 | 28.19 | N |
| ATOM | 1843 | CA | VAL A 242 | 18.284 | 42.335 | 33.552 | 1.00 | 28.55 | C |
| ATOM | 1844 | C | VAL A 242 | 17.117 | 41.409 | 33.563 | 1.00 | 28.88 | C |
| ATOM | 1845 | O | VAL A 242 | 17.198 | 40.314 | 33.053 | 1.00 | 28.92 | O |
| ATOM | 1846 | CB | VAL A 242 | 18.422 | 42.770 | 32.093 | 1.00 | 29.31 | C |
| ATOM | 1847 | CG1 | VAL A 242 | 17.165 | 43.549 | 31.647 | 1.00 | 27.90 | C |
| ATOM | 1848 | CG2 | VAL A 242 | 19.711 | 43.530 | 31.866 | 1.00 | 28.67 | C |
| ATOM | 1849 | N | ASP A 243 | 16.009 | 41.862 | 34.113 | 1.00 | 28.55 | N |
| ATOM | 1850 | CA | ASP A 243 | 14.766 | 41.103 | 34.052 | 1.00 | 27.62 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1851 | C | ASP | A | 243 | 14.121 | 41.396 | 32.709 | 1.00 | 27.45 | C |
| ATOM | 1852 | O | ASP | A | 243 | 13.579 | 42.480 | 32.452 | 1.00 | 25.90 | O |
| ATOM | 1853 | CB | ASP | A | 243 | 13.876 | 41.560 | 35.193 | 1.00 | 27.99 | C |
| ATOM | 1854 | CG | ASP | A | 243 | 12.509 | 40.945 | 35.177 | 1.00 | 29.40 | C |
| ATOM | 1855 | OD1 | ASP | A | 243 | 12.096 | 40.291 | 34.179 | 1.00 | 31.46 | O |
| ATOM | 1856 | OD2 | ASP | A | 243 | 11.747 | 41.110 | 36.161 | 1.00 | 32.65 | O |
| ATOM | 1857 | N | PHE | A | 244 | 14.180 | 40.419 | 31.825 | 1.00 | 28.27 | N |
| ATOM | 1858 | CA | PHE | A | 244 | 13.656 | 40.603 | 30.496 | 1.00 | 28.92 | C |
| ATOM | 1859 | C | PHE | A | 244 | 12.172 | 40.975 | 30.481 | 1.00 | 30.32 | C |
| ATOM | 1860 | O | PHE | A | 244 | 11.728 | 41.643 | 29.561 | 1.00 | 31.01 | O |
| ATOM | 1861 | CB | PHE | A | 244 | 13.900 | 39.369 | 29.657 | 1.00 | 29.32 | C |
| ATOM | 1862 | CG | PHE | A | 244 | 15.255 | 39.298 | 29.053 | 1.00 | 28.51 | C |
| ATOM | 1863 | CD1 | PHE | A | 244 | 16.397 | 39.628 | 29.775 | 1.00 | 31.29 | C |
| ATOM | 1864 | CD2 | PHE | A | 244 | 15.399 | 38.853 | 27.793 | 1.00 | 28.23 | C |
| ATOM | 1865 | CE1 | PHE | A | 244 | 17.649 | 39.535 | 29.196 | 1.00 | 29.39 | C |
| ATOM | 1866 | CE2 | PHE | A | 244 | 16.654 | 38.736 | 27.229 | 1.00 | 30.79 | C |
| ATOM | 1867 | CZ | PHE | A | 244 | 17.759 | 39.107 | 27.919 | 1.00 | 29.44 | C |
| ATOM | 1868 | N | ASP | A | 245 | 11.401 | 40.551 | 31.482 | 1.00 | 31.22 | N |
| ATOM | 1869 | CA | ASP | A | 245 | 10.007 | 40.913 | 31.544 | 1.00 | 31.40 | C |
| ATOM | 1870 | C | ASP | A | 245 | 9.770 | 42.349 | 32.032 | 1.00 | 31.91 | C |
| ATOM | 1871 | O | ASP | A | 245 | 8.704 | 42.891 | 31.786 | 1.00 | 30.40 | O |
| ATOM | 1872 | CB | ASP | A | 245 | 9.263 | 39.968 | 32.467 | 1.00 | 32.57 | C |
| ATOM | 1873 | CG | ASP | A | 245 | 9.292 | 38.546 | 31.988 | 1.00 | 33.29 | C |
| ATOM | 1874 | OD1 | ASP | A | 245 | 9.289 | 38.333 | 30.768 | 1.00 | 35.51 | O |
| ATOM | 1875 | OD2 | ASP | A | 245 | 9.348 | 37.577 | 32.764 | 1.00 | 35.50 | O |
| ATOM | 1876 | N | ASN | A | 246 | 10.735 | 42.954 | 32.731 | 1.00 | 32.07 | N |
| ATOM | 1877 | CA | ASN | A | 246 | 10.562 | 44.310 | 33.244 | 1.00 | 33.10 | C |
| ATOM | 1878 | C | ASN | A | 246 | 11.884 | 45.016 | 33.384 | 1.00 | 32.49 | C |
| ATOM | 1879 | O | ASN | A | 246 | 12.400 | 45.179 | 34.476 | 1.00 | 33.20 | O |
| ATOM | 1880 | CB | ASN | A | 246 | 9.873 | 44.296 | 34.603 | 1.00 | 33.31 | C |
| ATOM | 1881 | CG | ASN | A | 246 | 9.555 | 45.716 | 35.110 | 1.00 | 39.27 | C |
| ATOM | 1882 | OD1 | ASN | A | 246 | 9.331 | 46.678 | 34.313 | 1.00 | 43.28 | O |
| ATOM | 1883 | ND2 | ASN | A | 246 | 9.551 | 45.867 | 36.445 | 1.00 | 44.32 | N |
| ATOM | 1884 | N | PRO | A | 247 | 12.472 | 45.374 | 32.265 | 1.00 | 31.66 | N |
| ATOM | 1885 | CA | PRO | A | 247 | 13.822 | 45.936 | 32.263 | 1.00 | 31.26 | C |
| ATOM | 1886 | C | PRO | A | 247 | 13.924 | 47.298 | 32.933 | 1.00 | 31.58 | C |
| ATOM | 1887 | O | PRO | A | 247 | 13.185 | 48.211 | 32.629 | 1.00 | 31.85 | O |
| ATOM | 1888 | CB | PRO | A | 247 | 14.161 | 46.082 | 30.782 | 1.00 | 31.22 | C |
| ATOM | 1889 | CG | PRO | A | 247 | 13.017 | 45.510 | 30.022 | 1.00 | 31.05 | C |
| ATOM | 1890 | CD | PRO | A | 247 | 11.894 | 45.216 | 30.928 | 1.00 | 31.01 | C |
| ATOM | 1891 | N | ASP | A | 248 | 14.893 | 47.422 | 33.815 | 1.00 | 31.35 | N |
| ATOM | 1892 | CA | ASP | A | 248 | 15.161 | 48.643 | 34.467 | 1.00 | 31.48 | C |
| ATOM | 1893 | C | ASP | A | 248 | 16.222 | 49.413 | 33.650 | 1.00 | 31.23 | C |
| ATOM | 1894 | O | ASP | A | 248 | 17.422 | 49.217 | 33.784 | 1.00 | 30.76 | O |
| ATOM | 1895 | CB | ASP | A | 248 | 15.646 | 48.310 | 35.850 | 1.00 | 31.60 | C |
| ATOM | 1896 | CG | ASP | A | 248 | 15.745 | 49.504 | 36.720 | 1.00 | 33.62 | C |
| ATOM | 1897 | OD1 | ASP | A | 248 | 16.020 | 50.619 | 36.201 | 1.00 | 34.39 | O |
| ATOM | 1898 | OD2 | ASP | A | 248 | 15.578 | 49.395 | 37.949 | 1.00 | 38.39 | O |
| ATOM | 1899 | N | TYR | A | 249 | 15.764 | 50.285 | 32.783 | 1.00 | 31.95 | N |
| ATOM | 1900 | CA | TYR | A | 249 | 16.676 | 51.053 | 31.942 | 1.00 | 32.80 | C |
| ATOM | 1901 | C | TYR | A | 249 | 17.534 | 52.052 | 32.714 | 1.00 | 33.92 | C |
| ATOM | 1902 | O | TYR | A | 249 | 18.558 | 52.490 | 32.203 | 1.00 | 34.33 | O |
| ATOM | 1903 | CB | TYR | A | 249 | 15.906 | 51.732 | 30.825 | 1.00 | 32.56 | C |
| ATOM | 1904 | CG | TYR | A | 249 | 15.183 | 50.751 | 29.928 | 1.00 | 31.41 | C |
| ATOM | 1905 | CD1 | TYR | A | 249 | 15.859 | 49.695 | 29.316 | 1.00 | 30.27 | C |
| ATOM | 1906 | CD2 | TYR | A | 249 | 13.845 | 50.868 | 29.704 | 1.00 | 29.24 | C |
| ATOM | 1907 | CE1 | TYR | A | 249 | 15.205 | 48.814 | 28.478 | 1.00 | 29.30 | C |
| ATOM | 1908 | CE2 | TYR | A | 249 | 13.178 | 49.968 | 28.894 | 1.00 | 29.24 | C |
| ATOM | 1909 | CZ | TYR | A | 249 | 13.858 | 48.947 | 28.285 | 1.00 | 29.20 | C |
| ATOM | 1910 | OH | TYR | A | 249 | 13.173 | 48.078 | 27.452 | 1.00 | 29.69 | O |
| ATOM | 1911 | N | GLU | A | 250 | 17.155 | 52.369 | 33.952 | 1.00 | 34.69 | N |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1912 | CA | GLU | A | 250 | 17.994 | 53.202 | 34.789 | 1.00 | 35.66 | C |
| ATOM | 1913 | C | GLU | A | 250 | 19.249 | 52.494 | 35.235 | 1.00 | 34.69 | C |
| ATOM | 1914 | O | GLU | A | 250 | 20.313 | 53.077 | 35.207 | 1.00 | 34.29 | O |
| ATOM | 1915 | CB | GLU | A | 250 | 17.252 | 53.685 | 36.021 | 1.00 | 36.82 | C |
| ATOM | 1916 | CG | GLU | A | 250 | 16.115 | 54.609 | 35.650 | 1.00 | 41.99 | C |
| ATOM | 1917 | CD | GLU | A | 250 | 15.554 | 55.360 | 36.827 | 1.00 | 48.02 | C |
| ATOM | 1918 | OE1 | GLU | A | 250 | 16.114 | 55.275 | 37.949 | 1.00 | 53.95 | O |
| ATOM | 1919 | OE2 | GLU | A | 250 | 14.543 | 56.043 | 36.614 | 1.00 | 52.47 | O |
| ATOM | 1920 | N | ARG | A | 251 | 19.139 | 51.254 | 35.691 | 1.00 | 33.87 | N |
| ATOM | 1921 | CA | ARG | A | 251 | 20.335 | 50.550 | 36.088 | 1.00 | 33.26 | C |
| ATOM | 1922 | C | ARG | A | 251 | 21.013 | 49.992 | 34.873 | 1.00 | 32.36 | C |
| ATOM | 1923 | O | ARG | A | 251 | 22.210 | 49.914 | 34.849 | 1.00 | 32.79 | O |
| ATOM | 1924 | CB | ARG | A | 251 | 20.040 | 49.425 | 37.066 | 1.00 | 34.36 | C |
| ATOM | 1925 | CG | ARG | A | 251 | 19.476 | 49.895 | 38.425 | 1.00 | 36.13 | C |
| ATOM | 1926 | CD | ARG | A | 251 | 18.966 | 48.771 | 39.339 | 1.00 | 39.31 | C |
| ATOM | 1927 | NE | ARG | A | 251 | 20.052 | 47.860 | 39.733 | 1.00 | 42.09 | N |
| ATOM | 1928 | CZ | ARG | A | 251 | 19.890 | 46.563 | 39.964 | 1.00 | 41.90 | C |
| ATOM | 1929 | NH1 | ARG | A | 251 | 18.696 | 46.006 | 39.843 | 1.00 | 41.62 | N |
| ATOM | 1930 | NH2 | ARG | A | 251 | 20.932 | 45.815 | 40.296 | 1.00 | 41.98 | N |
| ATOM | 1931 | N | PHE | A | 252 | 20.272 | 49.654 | 33.825 | 1.00 | 31.66 | N |
| ATOM | 1932 | CA | PHE | A | 252 | 20.879 | 48.977 | 32.677 | 1.00 | 30.28 | C |
| ATOM | 1933 | C | PHE | A | 252 | 20.528 | 49.651 | 31.347 | 1.00 | 29.72 | C |
| ATOM | 1934 | O | PHE | A | 252 | 19.882 | 49.096 | 30.483 | 1.00 | 29.84 | O |
| ATOM | 1935 | CB | PHE | A | 252 | 20.420 | 47.531 | 32.675 | 1.00 | 29.99 | C |
| ATOM | 1936 | CG | PHE | A | 252 | 20.405 | 46.864 | 34.050 | 1.00 | 29.63 | C |
| ATOM | 1937 | CD1 | PHE | A | 252 | 21.562 | 46.717 | 34.796 | 1.00 | 29.74 | C |
| ATOM | 1938 | CD2 | PHE | A | 252 | 19.238 | 46.317 | 34.554 | 1.00 | 31.30 | C |
| ATOM | 1939 | CE1 | PHE | A | 252 | 21.546 | 46.067 | 36.039 | 1.00 | 30.44 | C |
| ATOM | 1940 | CE2 | PHE | A | 252 | 19.199 | 45.668 | 35.805 | 1.00 | 31.42 | C |
| ATOM | 1941 | CZ | PHE | A | 252 | 20.356 | 45.551 | 36.550 | 1.00 | 32.04 | C |
| ATOM | 1942 | N | PRO | A | 253 | 21.034 | 50.844 | 31.155 | 1.00 | 29.72 | N |
| ATOM | 1943 | CA | PRO | A | 253 | 20.607 | 51.662 | 30.022 | 1.00 | 28.89 | C |
| ATOM | 1944 | C | PRO | A | 253 | 20.953 | 50.996 | 28.689 | 1.00 | 29.46 | C |
| ATOM | 1945 | O | PRO | A | 253 | 20.166 | 51.061 | 27.722 | 1.00 | 28.81 | O |
| ATOM | 1946 | CB | PRO | A | 253 | 21.361 | 52.975 | 30.240 | 1.00 | 28.37 | C |
| ATOM | 1947 | CG | PRO | A | 253 | 22.543 | 52.614 | 31.155 | 1.00 | 27.97 | C |
| ATOM | 1948 | CD | PRO | A | 253 | 22.136 | 51.463 | 31.942 | 1.00 | 29.24 | C |
| ATOM | 1949 | N | ASN | A | 254 | 22.093 | 50.323 | 28.590 | 1.00 | 29.37 | N |
| ATOM | 1950 | CA | ASN | A | 254 | 22.401 | 49.742 | 27.274 | 1.00 | 28.85 | C |
| ATOM | 1951 | C | ASN | A | 254 | 21.547 | 48.529 | 26.902 | 1.00 | 28.28 | C |
| ATOM | 1952 | O | ASN | A | 254 | 21.663 | 47.970 | 25.794 | 1.00 | 27.47 | O |
| ATOM | 1953 | CB | ASN | A | 254 | 23.874 | 49.407 | 27.122 | 1.00 | 28.84 | C |
| ATOM | 1954 | CG | ASN | A | 254 | 24.745 | 50.654 | 26.996 | 1.00 | 29.96 | C |
| ATOM | 1955 | OD1 | ASN | A | 254 | 25.622 | 50.882 | 27.834 | 1.00 | 31.21 | O |
| ATOM | 1956 | ND2 | ASN | A | 254 | 24.531 | 51.443 | 25.931 | 1.00 | 29.17 | N |
| ATOM | 1957 | N | PHE | A | 255 | 20.687 | 48.091 | 27.797 | 1.00 | 27.30 | N |
| ATOM | 1958 | CA | PHE | A | 255 | 19.801 | 47.006 | 27.368 | 1.00 | 27.53 | C |
| ATOM | 1959 | C | PHE | A | 255 | 18.844 | 47.512 | 26.283 | 1.00 | 26.80 | C |
| ATOM | 1960 | O | PHE | A | 255 | 18.193 | 46.750 | 25.603 | 1.00 | 27.22 | O |
| ATOM | 1961 | CB | PHE | A | 255 | 19.015 | 46.448 | 28.538 | 1.00 | 27.48 | C |
| ATOM | 1962 | CG | PHE | A | 255 | 18.282 | 45.250 | 28.198 | 1.00 | 26.63 | C |
| ATOM | 1963 | CD1 | PHE | A | 255 | 18.950 | 44.073 | 27.998 | 1.00 | 29.74 | C |
| ATOM | 1964 | CD2 | PHE | A | 255 | 16.935 | 45.288 | 28.039 | 1.00 | 26.29 | C |
| ATOM | 1965 | CE1 | PHE | A | 255 | 18.273 | 42.947 | 27.681 | 1.00 | 29.50 | C |
| ATOM | 1966 | CE2 | PHE | A | 255 | 16.261 | 44.192 | 27.692 | 1.00 | 26.21 | C |
| ATOM | 1967 | CZ | PHE | A | 255 | 16.917 | 43.012 | 27.518 | 1.00 | 30.10 | C |
| ATOM | 1968 | N | GLN | A | 256 | 18.776 | 48.818 | 26.125 | 1.00 | 26.57 | N |
| ATOM | 1969 | CA | GLN | A | 256 | 17.918 | 49.429 | 25.137 | 1.00 | 26.55 | C |
| ATOM | 1970 | C | GLN | A | 256 | 18.522 | 49.253 | 23.745 | 1.00 | 26.46 | C |
| ATOM | 1971 | O | GLN | A | 256 | 17.881 | 49.560 | 22.771 | 1.00 | 24.39 | O |
| ATOM | 1972 | CB | GLN | A | 256 | 17.756 | 50.933 | 25.423 | 1.00 | 26.18 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1973 | CG | GLN | A | 256 | 16.656 | 51.226 | 26.406 | 1.00 | 28.72 | C |
| ATOM | 1974 | CD | GLN | A | 256 | 16.721 | 52.636 | 27.028 | 1.00 | 29.64 | C |
| ATOM | 1975 | OE1 | GLN | A | 256 | 15.737 | 53.358 | 27.005 | 1.00 | 32.56 | O |
| ATOM | 1976 | NE2 | GLN | A | 256 | 17.861 | 52.999 | 27.590 | 1.00 | 26.88 | N |
| ATOM | 1977 | N | ASN | A | 257 | 19.774 | 48.809 | 23.694 | 1.00 | 27.86 | N |
| ATOM | 1978 | CA | ASN | A | 257 | 20.509 | 48.611 | 22.452 | 1.00 | 29.22 | C |
| ATOM | 1979 | C | ASN | A | 257 | 20.733 | 47.143 | 22.116 | 1.00 | 30.46 | C |
| ATOM | 1980 | O | ASN | A | 257 | 21.399 | 46.855 | 21.132 | 1.00 | 32.28 | O |
| ATOM | 1981 | CB | ASN | A | 257 | 21.897 | 49.232 | 22.510 | 1.00 | 28.50 | C |
| ATOM | 1982 | CG | ASN | A | 257 | 21.878 | 50.666 | 22.890 | 1.00 | 29.30 | C |
| ATOM | 1983 | OD1 | ASN | A | 257 | 22.329 | 51.025 | 23.989 | 1.00 | 27.33 | O |
| ATOM | 1984 | ND2 | ASN | A | 257 | 21.382 | 51.523 | 21.982 | 1.00 | 25.68 | N |
| ATOM | 1985 | N | VAL | A | 258 | 20.200 | 46.213 | 22.900 | 1.00 | 31.51 | N |
| ATOM | 1986 | CA | VAL | A | 258 | 20.432 | 44.791 | 22.623 | 1.00 | 32.54 | C |
| ATOM | 1987 | C | VAL | A | 258 | 19.674 | 44.295 | 21.386 | 1.00 | 32.39 | C |
| ATOM | 1988 | O | VAL | A | 258 | 18.543 | 44.766 | 21.081 | 1.00 | 32.29 | O |
| ATOM | 1989 | CB | VAL | A | 258 | 20.050 | 43.937 | 23.841 | 1.00 | 33.12 | C |
| ATOM | 1990 | CG1 | VAL | A | 258 | 18.546 | 43.818 | 23.986 | 1.00 | 32.40 | C |
| ATOM | 1991 | CG2 | VAL | A | 258 | 20.646 | 42.566 | 23.686 | 1.00 | 36.78 | C |
| ATOM | 1992 | N | VAL | A | 259 | 20.302 | 43.386 | 20.654 | 1.00 | 32.45 | N |
| ATOM | 1993 | CA | VAL | A | 259 | 19.682 | 42.796 | 19.448 | 1.00 | 32.96 | C |
| ATOM | 1994 | C | VAL | A | 259 | 19.943 | 41.301 | 19.391 | 1.00 | 33.08 | C |
| ATOM | 1995 | O | VAL | A | 259 | 21.074 | 40.878 | 19.351 | 1.00 | 33.50 | O |
| ATOM | 1996 | CB | VAL | A | 259 | 20.269 | 43.401 | 18.172 | 1.00 | 33.19 | C |
| ATOM | 1997 | CG1 | VAL | A | 259 | 19.625 | 42.771 | 16.962 | 1.00 | 34.73 | C |
| ATOM | 1998 | CG2 | VAL | A | 259 | 20.054 | 44.901 | 18.143 | 1.00 | 32.25 | C |
| ATOM | 1999 | N | GLY | A | 260 | 18.902 | 40.491 | 19.406 | 1.00 | 33.70 | N |
| ATOM | 2000 | CA | GLY | A | 260 | 19.091 | 39.052 | 19.368 | 1.00 | 34.16 | C |
| ATOM | 2001 | C | GLY | A | 260 | 19.036 | 38.327 | 18.014 | 1.00 | 33.92 | C |
| ATOM | 2002 | O | GLY | A | 260 | 18.655 | 38.891 | 16.975 | 1.00 | 33.59 | O |
| ATOM | 2003 | N | TYR | A | 261 | 19.469 | 37.071 | 18.052 | 1.00 | 33.14 | N |
| ATOM | 2004 | CA | TYR | A | 261 | 19.375 | 36.157 | 16.938 | 1.00 | 33.55 | C |
| ATOM | 2005 | C | TYR | A | 261 | 18.439 | 35.095 | 17.489 | 1.00 | 33.41 | C |
| ATOM | 2006 | O | TYR | A | 261 | 18.700 | 34.542 | 18.561 | 1.00 | 33.67 | O |
| ATOM | 2007 | CB | TYR | A | 261 | 20.715 | 35.508 | 16.657 | 1.00 | 33.81 | C |
| ATOM | 2008 | CG | TYR | A | 261 | 21.758 | 36.416 | 16.061 | 1.00 | 36.80 | C |
| ATOM | 2009 | CD1 | TYR | A | 261 | 21.886 | 36.545 | 14.694 | 1.00 | 42.37 | C |
| ATOM | 2010 | CD2 | TYR | A | 261 | 22.602 | 37.139 | 16.851 | 1.00 | 38.31 | C |
| ATOM | 2011 | CE1 | TYR | A | 261 | 22.823 | 37.378 | 14.139 | 1.00 | 43.02 | C |
| ATOM | 2012 | CE2 | TYR | A | 261 | 23.556 | 37.938 | 16.312 | 1.00 | 40.85 | C |
| ATOM | 2013 | CZ | TYR | A | 261 | 23.660 | 38.058 | 14.955 | 1.00 | 42.50 | C |
| ATOM | 2014 | OH | TYR | A | 261 | 24.617 | 38.865 | 14.414 | 1.00 | 45.43 | O |
| ATOM | 2015 | N | GLU | A | 262 | 17.322 | 34.832 | 16.834 | 1.00 | 32.71 | N |
| ATOM | 2016 | CA | GLU | A | 262 | 16.394 | 33.886 | 17.438 | 1.00 | 32.21 | C |
| ATOM | 2017 | C | GLU | A | 262 | 15.975 | 32.768 | 16.508 | 1.00 | 30.89 | C |
| ATOM | 2018 | O | GLU | A | 262 | 16.180 | 32.819 | 15.294 | 1.00 | 30.63 | O |
| ATOM | 2019 | CB | GLU | A | 262 | 15.196 | 34.613 | 18.049 | 1.00 | 32.16 | C |
| ATOM | 2020 | CG | GLU | A | 262 | 13.968 | 34.753 | 17.210 | 1.00 | 30.84 | C |
| ATOM | 2021 | CD | GLU | A | 262 | 12.818 | 35.380 | 17.992 | 1.00 | 31.21 | C |
| ATOM | 2022 | OE1 | GLU | A | 262 | 12.761 | 36.612 | 18.108 | 1.00 | 34.58 | O |
| ATOM | 2023 | OE2 | GLU | A | 262 | 11.962 | 34.663 | 18.504 | 1.00 | 29.56 | O |
| ATOM | 2024 | N | THR | A | 263 | 15.447 | 31.746 | 17.133 | 1.00 | 28.97 | N |
| ATOM | 2025 | CA | THR | A | 263 | 14.941 | 30.587 | 16.447 | 1.00 | 28.44 | C |
| ATOM | 2026 | C | THR | A | 263 | 14.080 | 29.743 | 17.387 | 1.00 | 27.24 | C |
| ATOM | 2027 | O | THR | A | 263 | 14.088 | 29.893 | 18.620 | 1.00 | 26.43 | O |
| ATOM | 2028 | CB | THR | A | 263 | 16.093 | 29.746 | 15.902 | 1.00 | 28.50 | C |
| ATOM | 2029 | OG1 | THR | A | 263 | 15.592 | 28.798 | 14.964 | 1.00 | 27.18 | O |
| ATOM | 2030 | CG2 | THR | A | 263 | 16.697 | 28.854 | 16.975 | 1.00 | 28.63 | C |
| ATOM | 2031 | N | VAL | A | 264 | 13.306 | 28.887 | 16.776 | 1.00 | 27.22 | N |
| ATOM | 2032 | CA | VAL | A | 264 | 12.509 | 27.942 | 17.497 | 1.00 | 28.49 | C |
| ATOM | 2033 | C | VAL | A | 264 | 12.925 | 26.576 | 17.022 | 1.00 | 29.10 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2034 | O | VAL | A | 264 | 12.876 | 26.279 | 15.828 | 1.00 | 28.47 | O |
| ATOM | 2035 | CB | VAL | A | 264 | 11.025 | 28.126 | 17.252 | 1.00 | 29.23 | C |
| ATOM | 2036 | CG1 | VAL | A | 264 | 10.259 | 26.871 | 17.767 | 1.00 | 29.07 | C |
| ATOM | 2037 | CG2 | VAL | A | 264 | 10.520 | 29.431 | 17.973 | 1.00 | 28.52 | C |
| ATOM | 2038 | N | VAL | A | 265 | 13.401 | 25.763 | 17.954 | 1.00 | 29.56 | N |
| ATOM | 2039 | CA | VAL | A | 265 | 13.806 | 24.413 | 17.594 | 1.00 | 29.83 | C |
| ATOM | 2040 | C | VAL | A | 265 | 12.785 | 23.404 | 18.039 | 1.00 | 29.63 | C |
| ATOM | 2041 | O | VAL | A | 265 | 12.188 | 23.544 | 19.105 | 1.00 | 29.93 | O |
| ATOM | 2042 | CB | VAL | A | 265 | 15.197 | 24.015 | 18.203 | 1.00 | 29.88 | C |
| ATOM | 2043 | CG1 | VAL | A | 265 | 16.281 | 24.883 | 17.589 | 1.00 | 32.24 | C |
| ATOM | 2044 | CG2 | VAL | A | 265 | 15.234 | 24.114 | 19.712 | 1.00 | 26.80 | C |
| ATOM | 2045 | N | GLY | A | 266 | 12.642 | 22.371 | 17.226 | 1.00 | 28.96 | N |
| ATOM | 2046 | CA | GLY | A | 266 | 11.770 | 21.268 | 17.513 | 1.00 | 28.86 | C |
| ATOM | 2047 | C | GLY | A | 266 | 12.463 | 19.909 | 17.428 | 1.00 | 28.32 | C |
| ATOM | 2048 | O | GLY | A | 266 | 13.656 | 19.804 | 17.215 | 1.00 | 28.58 | O |
| ATOM | 2049 | N | PRO | A | 267 | 11.696 | 18.852 | 17.581 | 1.00 | 28.06 | N |
| ATOM | 2050 | CA | PRO | A | 267 | 12.278 | 17.505 | 17.565 | 1.00 | 28.37 | C |
| ATOM | 2051 | C | PRO | A | 267 | 13.148 | 17.313 | 16.360 | 1.00 | 28.01 | C |
| ATOM | 2052 | O | PRO | A | 267 | 12.674 | 17.573 | 15.265 | 1.00 | 28.36 | O |
| ATOM | 2053 | CB | PRO | A | 267 | 11.047 | 16.582 | 17.482 | 1.00 | 27.55 | C |
| ATOM | 2054 | CG | PRO | A | 267 | 10.000 | 17.278 | 18.220 | 1.00 | 28.05 | C |
| ATOM | 2055 | CD | PRO | A | 267 | 10.237 | 18.817 | 17.827 | 1.00 | 28.28 | C |
| ATOM | 2056 | N | GLY | A | 268 | 14.392 | 16.878 | 16.562 | 1.00 | 27.37 | N |
| ATOM | 2057 | CA | GLY | A | 268 | 15.273 | 16.605 | 15.453 | 1.00 | 25.78 | C |
| ATOM | 2058 | C | GLY | A | 268 | 16.231 | 17.726 | 15.175 | 1.00 | 25.51 | C |
| ATOM | 2059 | O | GLY | A | 268 | 17.237 | 17.508 | 14.519 | 1.00 | 26.07 | O |
| ATOM | 2060 | N | ASP | A | 269 | 15.957 | 18.928 | 15.653 | 1.00 | 25.79 | N |
| ATOM | 2061 | CA | ASP | A | 269 | 16.835 | 20.044 | 15.354 | 1.00 | 25.78 | C |
| ATOM | 2062 | C | ASP | A | 269 | 17.996 | 20.091 | 16.377 | 1.00 | 26.28 | C |
| ATOM | 2063 | O | ASP | A | 269 | 17.848 | 19.689 | 17.549 | 1.00 | 26.27 | O |
| ATOM | 2064 | CB | ASP | A | 269 | 16.106 | 21.376 | 15.504 | 1.00 | 26.89 | C |
| ATOM | 2065 | CG | ASP | A | 269 | 14.898 | 21.583 | 14.603 | 1.00 | 25.99 | C |
| ATOM | 2066 | OD1 | ASP | A | 269 | 14.745 | 20.966 | 13.562 | 1.00 | 28.50 | O |
| ATOM | 2067 | OD2 | ASP | A | 269 | 14.065 | 22.495 | 14.853 | 1.00 | 29.93 | O |
| ATOM | 2068 | N | VAL | A | 270 | 19.128 | 20.632 | 15.937 | 1.00 | 26.28 | N |
| ATOM | 2069 | CA | VAL | A | 270 | 20.291 | 20.847 | 16.775 | 1.00 | 26.03 | C |
| ATOM | 2070 | C | VAL | A | 270 | 20.780 | 22.271 | 16.628 | 1.00 | 26.03 | C |
| ATOM | 2071 | O | VAL | A | 270 | 21.123 | 22.727 | 15.547 | 1.00 | 25.72 | O |
| ATOM | 2072 | CB | VAL | A | 270 | 21.414 | 19.938 | 16.381 | 1.00 | 25.76 | C |
| ATOM | 2073 | CG1 | VAL | A | 270 | 22.675 | 20.325 | 17.113 | 1.00 | 26.27 | C |
| ATOM | 2074 | CG2 | VAL | A | 270 | 21.060 | 18.546 | 16.735 | 1.00 | 25.93 | C |
| ATOM | 2075 | N | LEU | A | 271 | 20.809 | 22.987 | 17.730 | 1.00 | 26.47 | N |
| ATOM | 2076 | CA | LEU | A | 271 | 21.257 | 24.364 | 17.713 | 1.00 | 26.42 | C |
| ATOM | 2077 | C | LEU | A | 271 | 22.673 | 24.422 | 18.228 | 1.00 | 27.12 | C |
| ATOM | 2078 | O | LEU | A | 271 | 22.973 | 23.936 | 19.310 | 1.00 | 26.82 | O |
| ATOM | 2079 | CB | LEU | A | 271 | 20.372 | 25.235 | 18.570 | 1.00 | 26.20 | C |
| ATOM | 2080 | CG | LEU | A | 271 | 20.935 | 26.646 | 18.783 | 1.00 | 27.91 | C |
| ATOM | 2081 | CD1 | LEU | A | 271 | 20.962 | 27.396 | 17.500 | 1.00 | 27.86 | C |
| ATOM | 2082 | CD2 | LEU | A | 271 | 20.100 | 27.425 | 19.789 | 1.00 | 29.16 | C |
| ATOM | 2083 | N | TYR | A | 272 | 23.563 | 24.980 | 17.423 | 1.00 | 27.82 | N |
| ATOM | 2084 | CA | TYR | A | 272 | 24.913 | 25.201 | 17.873 | 1.00 | 27.79 | C |
| ATOM | 2085 | C | TYR | A | 272 | 24.918 | 26.494 | 18.662 | 1.00 | 26.67 | C |
| ATOM | 2086 | O | TYR | A | 272 | 24.660 | 27.528 | 18.117 | 1.00 | 27.22 | O |
| ATOM | 2087 | CB | TYR | A | 272 | 25.898 | 25.325 | 16.693 | 1.00 | 27.26 | C |
| ATOM | 2088 | CG | TYR | A | 272 | 27.296 | 25.785 | 17.124 | 1.00 | 28.18 | C |
| ATOM | 2089 | CD1 | TYR | A | 272 | 27.924 | 25.237 | 18.221 | 1.00 | 28.32 | C |
| ATOM | 2090 | CD2 | TYR | A | 272 | 27.973 | 26.784 | 16.435 | 1.00 | 29.06 | C |
| ATOM | 2091 | CE1 | TYR | A | 272 | 29.169 | 25.653 | 18.600 | 1.00 | 28.29 | C |
| ATOM | 2092 | CE2 | TYR | A | 272 | 29.232 | 27.188 | 16.805 | 1.00 | 27.19 | C |
| ATOM | 2093 | CZ | TYR | A | 272 | 29.821 | 26.632 | 17.903 | 1.00 | 27.41 | C |
| ATOM | 2094 | OH | TYR | A | 272 | 31.081 | 27.026 | 18.322 | 1.00 | 24.66 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2095 | N | ILE | A | 273 | 25.237 | 26.418 | 19.934 | 1.00 | 26.87 | N |
| ATOM | 2096 | CA | ILE | A | 273 | 25.381 | 27.591 | 20.810 | 1.00 | 26.89 | C |
| ATOM | 2097 | C | ILE | A | 273 | 26.841 | 27.751 | 21.182 | 1.00 | 27.37 | C |
| ATOM | 2098 | O | ILE | A | 273 | 27.359 | 27.049 | 22.056 | 1.00 | 27.62 | O |
| ATOM | 2099 | CB | ILE | A | 273 | 24.647 | 27.422 | 22.085 | 1.00 | 26.74 | C |
| ATOM | 2100 | CG1 | ILE | A | 273 | 23.182 | 27.185 | 21.799 | 1.00 | 25.89 | C |
| ATOM | 2101 | CG2 | ILE | A | 273 | 24.852 | 28.675 | 22.941 | 1.00 | 26.79 | C |
| ATOM | 2102 | CD1 | ILE | A | 273 | 22.338 | 27.108 | 23.065 | 1.00 | 25.37 | C |
| ATOM | 2103 | N | PRO | A | 274 | 27.491 | 28.681 | 20.515 | 1.00 | 27.39 | N |
| ATOM | 2104 | CA | PRO | A | 274 | 28.923 | 28.871 | 20.601 | 1.00 | 27.76 | C |
| ATOM | 2105 | C | PRO | A | 274 | 29.287 | 29.415 | 21.934 | 1.00 | 27.42 | C |
| ATOM | 2106 | O | PRO | A | 274 | 28.483 | 30.135 | 22.518 | 1.00 | 26.71 | O |
| ATOM | 2107 | CB | PRO | A | 274 | 29.250 | 29.840 | 19.426 | 1.00 | 27.60 | C |
| ATOM | 2108 | CG | PRO | A | 274 | 27.980 | 30.107 | 18.741 | 1.00 | 28.16 | C |
| ATOM | 2109 | CD | PRO | A | 274 | 26.876 | 29.504 | 19.497 | 1.00 | 28.21 | C |
| ATOM | 2110 | N | MET | A | 275 | 30.467 | 29.017 | 22.394 | 1.00 | 27.88 | N |
| ATOM | 2111 | CA | MET | A | 275 | 30.979 | 29.346 | 23.717 | 1.00 | 28.91 | C |
| ATOM | 2112 | C | MET | A | 275 | 30.974 | 30.849 | 23.919 | 1.00 | 28.27 | C |
| ATOM | 2113 | O | MET | A | 275 | 31.284 | 31.589 | 23.000 | 1.00 | 27.69 | O |
| ATOM | 2114 | CB | MET | A | 275 | 32.365 | 28.808 | 23.869 | 1.00 | 29.00 | C |
| ATOM | 2115 | CG | MET | A | 275 | 32.861 | 28.842 | 25.313 | 1.00 | 34.03 | C |
| ATOM | 2116 | SD | MET | A | 275 | 34.499 | 28.084 | 25.455 | 1.00 | 39.22 | S |
| ATOM | 2117 | CE | MET | A | 275 | 35.200 | 28.479 | 23.871 | 1.00 | 36.40 | C |
| ATOM | 2118 | N | TYR | A | 276 | 30.531 | 31.294 | 25.086 | 1.00 | 27.79 | N |
| ATOM | 2119 | CA | TYR | A | 276 | 30.472 | 32.746 | 25.389 | 1.00 | 29.16 | C |
| ATOM | 2120 | C | TYR | A | 276 | 29.267 | 33.465 | 24.802 | 1.00 | 27.80 | C |
| ATOM | 2121 | O | TYR | A | 276 | 29.076 | 34.609 | 25.107 | 1.00 | 28.35 | O |
| ATOM | 2122 | CB | TYR | A | 276 | 31.779 | 33.506 | 24.974 | 1.00 | 29.63 | C |
| ATOM | 2123 | CG | TYR | A | 276 | 32.918 | 33.207 | 25.897 | 1.00 | 34.37 | C |
| ATOM | 2124 | CD1 | TYR | A | 276 | 32.966 | 33.783 | 27.146 | 1.00 | 38.52 | C |
| ATOM | 2125 | CD2 | TYR | A | 276 | 33.934 | 32.306 | 25.547 | 1.00 | 39.45 | C |
| ATOM | 2126 | CE1 | TYR | A | 276 | 33.955 | 33.493 | 28.022 | 1.00 | 39.83 | C |
| ATOM | 2127 | CE2 | TYR | A | 276 | 34.965 | 32.015 | 26.449 | 1.00 | 42.05 | C |
| ATOM | 2128 | CZ | TYR | A | 276 | 34.954 | 32.609 | 27.685 | 1.00 | 42.46 | C |
| ATOM | 2129 | OH | TYR | A | 276 | 35.949 | 32.343 | 28.624 | 1.00 | 48.60 | O |
| ATOM | 2130 | N | TRP | A | 277 | 28.468 | 32.830 | 23.951 | 1.00 | 27.45 | N |
| ATOM | 2131 | CA | TRP | A | 277 | 27.271 | 33.485 | 23.419 | 1.00 | 26.19 | C |
| ATOM | 2132 | C | TRP | A | 277 | 26.160 | 33.442 | 24.424 | 1.00 | 25.93 | C |
| ATOM | 2133 | O | TRP | A | 277 | 25.882 | 32.409 | 24.973 | 1.00 | 26.84 | O |
| ATOM | 2134 | CB | TRP | A | 277 | 26.796 | 32.826 | 22.130 | 1.00 | 26.07 | C |
| ATOM | 2135 | CG | TRP | A | 277 | 27.525 | 33.276 | 20.957 | 1.00 | 24.33 | C |
| ATOM | 2136 | CD1 | TRP | A | 277 | 28.862 | 33.118 | 20.731 | 1.00 | 24.81 | C |
| ATOM | 2137 | CD2 | TRP | A | 277 | 26.995 | 33.935 | 19.821 | 1.00 | 23.88 | C |
| ATOM | 2138 | NE1 | TRP | A | 277 | 29.204 | 33.674 | 19.531 | 1.00 | 24.86 | N |
| ATOM | 2139 | CE2 | TRP | A | 277 | 28.073 | 34.182 | 18.944 | 1.00 | 24.16 | C |
| ATOM | 2140 | CE3 | TRP | A | 277 | 25.727 | 34.398 | 19.464 | 1.00 | 25.16 | C |
| ATOM | 2141 | CZ2 | TRP | A | 277 | 27.923 | 34.858 | 17.747 | 1.00 | 23.53 | C |
| ATOM | 2142 | CZ3 | TRP | A | 277 | 25.579 | 35.064 | 18.250 | 1.00 | 25.92 | C |
| ATOM | 2143 | CH2 | TRP | A | 277 | 26.679 | 35.292 | 17.414 | 1.00 | 24.81 | C |
| ATOM | 2144 | N | TRP | A | 278 | 25.516 | 34.566 | 24.673 | 1.00 | 26.34 | N |
| ATOM | 2145 | CA | TRP | A | 278 | 24.408 | 34.623 | 25.625 | 1.00 | 26.96 | C |
| ATOM | 2146 | C | TRP | A | 278 | 23.229 | 33.847 | 25.050 | 1.00 | 27.33 | C |
| ATOM | 2147 | O | TRP | A | 278 | 23.021 | 33.846 | 23.847 | 1.00 | 27.18 | O |
| ATOM | 2148 | CB | TRP | A | 278 | 23.952 | 36.062 | 25.838 | 1.00 | 26.87 | C |
| ATOM | 2149 | CG | TRP | A | 278 | 24.965 | 36.916 | 26.455 | 1.00 | 27.61 | C |
| ATOM | 2150 | CD1 | TRP | A | 278 | 25.997 | 37.558 | 25.833 | 1.00 | 28.27 | C |
| ATOM | 2151 | CD2 | TRP | A | 278 | 25.065 | 37.228 | 27.830 | 1.00 | 25.52 | C |
| ATOM | 2152 | NE1 | TRP | A | 278 | 26.731 | 38.261 | 26.753 | 1.00 | 28.77 | N |
| ATOM | 2153 | CE2 | TRP | A | 278 | 26.164 | 38.072 | 27.991 | 1.00 | 29.02 | C |
| ATOM | 2154 | CE3 | TRP | A | 278 | 24.303 | 36.915 | 28.942 | 1.00 | 26.86 | C |
| ATOM | 2155 | CZ2 | TRP | A | 278 | 26.541 | 38.563 | 29.224 | 1.00 | 28.96 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2156 | CZ3 | TRP | A | 278 | 24.676 | 37.402 | 30.157 | 1.00 | 29.86 | C |
| ATOM | 2157 | CH2 | TRP | A | 278 | 25.780 | 38.224 | 30.293 | 1.00 | 27.89 | C |
| ATOM | 2158 | N | HIS | A | 279 | 22.455 | 33.193 | 25.890 | 1.00 | 27.47 | N |
| ATOM | 2159 | CA | HIS | A | 279 | 21.263 | 32.554 | 25.380 | 1.00 | 28.50 | C |
| ATOM | 2160 | C | HIS | A | 279 | 20.158 | 32.574 | 26.403 | 1.00 | 28.09 | C |
| ATOM | 2161 | O | HIS | A | 279 | 20.420 | 32.445 | 27.584 | 1.00 | 29.26 | O |
| ATOM | 2162 | CB | HIS | A | 279 | 21.528 | 31.112 | 24.899 | 1.00 | 28.46 | C |
| ATOM | 2163 | CG | HIS | A | 279 | 22.339 | 30.278 | 25.838 | 1.00 | 30.29 | C |
| ATOM | 2164 | ND1 | HIS | A | 279 | 23.712 | 30.381 | 25.928 | 1.00 | 31.17 | N |
| ATOM | 2165 | CD2 | HIS | A | 279 | 21.984 | 29.270 | 26.673 | 1.00 | 31.89 | C |
| ATOM | 2166 | CE1 | HIS | A | 279 | 24.161 | 29.484 | 26.790 | 1.00 | 31.48 | C |
| ATOM | 2167 | NE2 | HIS | A | 279 | 23.136 | 28.810 | 27.271 | 1.00 | 30.92 | N |
| ATOM | 2168 | N | HIS | A | 280 | 18.942 | 32.764 | 25.916 | 1.00 | 28.12 | N |
| ATOM | 2169 | CA | HIS | A | 280 | 17.713 | 32.827 | 26.695 | 1.00 | 28.50 | C |
| ATOM | 2170 | C | HIS | A | 280 | 16.884 | 31.731 | 26.071 | 1.00 | 28.78 | C |
| ATOM | 2171 | O | HIS | A | 280 | 16.739 | 31.709 | 24.851 | 1.00 | 29.67 | O |
| ATOM | 2172 | CB | HIS | A | 280 | 17.069 | 34.196 | 26.498 | 1.00 | 27.71 | C |
| ATOM | 2173 | CG | HIS | A | 280 | 15.600 | 34.223 | 26.727 | 1.00 | 29.69 | C |
| ATOM | 2174 | ND1 | HIS | A | 280 | 15.021 | 34.905 | 27.782 | 1.00 | 31.66 | N |
| ATOM | 2175 | CD2 | HIS | A | 280 | 14.579 | 33.648 | 26.047 | 1.00 | 31.45 | C |
| ATOM | 2176 | CE1 | HIS | A | 280 | 13.710 | 34.743 | 27.738 | 1.00 | 30.66 | C |
| ATOM | 2177 | NE2 | HIS | A | 280 | 13.415 | 33.985 | 26.696 | 1.00 | 31.28 | N |
| ATOM | 2178 | N | ILE | A | 281 | 16.346 | 30.814 | 26.860 | 1.00 | 29.23 | N |
| ATOM | 2179 | CA | ILE | A | 281 | 15.651 | 29.652 | 26.294 | 1.00 | 29.56 | C |
| ATOM | 2180 | C | ILE | A | 281 | 14.311 | 29.497 | 26.922 | 1.00 | 30.16 | C |
| ATOM | 2181 | O | ILE | A | 281 | 14.190 | 29.517 | 28.135 | 1.00 | 30.14 | O |
| ATOM | 2182 | CB | ILE | A | 281 | 16.478 | 28.409 | 26.516 | 1.00 | 29.69 | C |
| ATOM | 2183 | CG1 | ILE | A | 281 | 17.707 | 28.491 | 25.628 | 1.00 | 30.69 | C |
| ATOM | 2184 | CG2 | ILE | A | 281 | 15.686 | 27.119 | 26.172 | 1.00 | 28.22 | C |
| ATOM | 2185 | CD1 | ILE | A | 281 | 18.689 | 27.534 | 25.980 | 1.00 | 33.11 | C |
| ATOM | 2186 | N | GLU | A | 282 | 13.280 | 29.380 | 26.103 | 1.00 | 31.22 | N |
| ATOM | 2187 | CA | GLU | A | 282 | 11.931 | 29.278 | 26.665 | 1.00 | 31.99 | C |
| ATOM | 2188 | C | GLU | A | 282 | 11.123 | 28.182 | 26.007 | 1.00 | 31.79 | C |
| ATOM | 2189 | O | GLU | A | 282 | 11.131 | 28.021 | 24.806 | 1.00 | 32.77 | O |
| ATOM | 2190 | CB | GLU | A | 282 | 11.200 | 30.638 | 26.618 | 1.00 | 32.16 | C |
| ATOM | 2191 | CG | GLU | A | 282 | 11.017 | 31.265 | 25.253 | 1.00 | 33.49 | C |
| ATOM | 2192 | CD | GLU | A | 282 | 10.378 | 32.663 | 25.313 | 1.00 | 36.22 | C |
| ATOM | 2193 | OE1 | GLU | A | 282 | 10.879 | 33.552 | 26.043 | 1.00 | 38.20 | O |
| ATOM | 2194 | OE2 | GLU | A | 282 | 9.380 | 32.898 | 24.603 | 1.00 | 38.15 | O |
| ATOM | 2195 | N | SER | A | 283 | 10.454 | 27.392 | 26.827 | 1.00 | 31.81 | N |
| ATOM | 2196 | CA | SER | A | 283 | 9.592 | 26.333 | 26.331 | 1.00 | 30.79 | C |
| ATOM | 2197 | C | SER | A | 283 | 8.245 | 26.975 | 25.950 | 1.00 | 30.98 | C |
| ATOM | 2198 | O | SER | A | 283 | 7.635 | 27.640 | 26.780 | 1.00 | 30.36 | O |
| ATOM | 2199 | CB | SER | A | 283 | 9.430 | 25.305 | 27.424 | 1.00 | 30.62 | C |
| ATOM | 2200 | OG | SER | A | 283 | 10.586 | 24.463 | 27.496 | 1.00 | 29.45 | O |
| ATOM | 2201 | N | LEU | A | 284 | 7.776 | 26.790 | 24.709 | 1.00 | 31.06 | N |
| ATOM | 2202 | CA | LEU | A | 284 | 6.587 | 27.504 | 24.270 | 1.00 | 31.43 | C |
| ATOM | 2203 | C | LEU | A | 284 | 5.398 | 27.390 | 25.204 | 1.00 | 31.82 | C |
| ATOM | 2204 | O | LEU | A | 284 | 5.137 | 26.333 | 25.776 | 1.00 | 31.15 | O |
| ATOM | 2205 | CB | LEU | A | 284 | 6.156 | 27.098 | 22.895 | 1.00 | 31.75 | C |
| ATOM | 2206 | CG | LEU | A | 284 | 7.223 | 27.187 | 21.829 | 1.00 | 33.11 | C |
| ATOM | 2207 | CD1 | LEU | A | 284 | 6.571 | 27.388 | 20.478 | 1.00 | 33.62 | C |
| ATOM | 2208 | CD2 | LEU | A | 284 | 8.170 | 28.270 | 22.142 | 1.00 | 32.91 | C |
| ATOM | 2209 | N | LEU | A | 285 | 4.701 | 28.512 | 25.355 | 1.00 | 32.74 | N |
| ATOM | 2210 | CA | LEU | A | 285 | 3.481 | 28.564 | 26.147 | 1.00 | 34.35 | C |
| ATOM | 2211 | C | LEU | A | 285 | 2.502 | 27.591 | 25.540 | 1.00 | 34.74 | C |
| ATOM | 2212 | O | LEU | A | 285 | 2.375 | 27.510 | 24.332 | 1.00 | 34.70 | O |
| ATOM | 2213 | CB | LEU | A | 285 | 2.863 | 29.946 | 26.094 | 1.00 | 34.26 | C |
| ATOM | 2214 | CG | LEU | A | 285 | 3.729 | 31.060 | 26.638 | 1.00 | 34.74 | C |
| ATOM | 2215 | CD1 | LEU | A | 285 | 3.183 | 32.369 | 26.160 | 1.00 | 34.14 | C |
| ATOM | 2216 | CD2 | LEU | A | 285 | 3.780 | 30.970 | 28.136 | 1.00 | 34.97 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2217 | N | ASN A 286 | 1.838 | 26.829 | 26.380 | 1.00 | 35.89 | | N |
| ATOM | 2218 | CA | ASN A 286 | 0.841 | 25.863 | 25.896 | 1.00 | 37.12 | | C |
| ATOM | 2219 | C | ASN A 286 | 1.363 | 24.809 | 24.909 | 1.00 | 36.14 | | C |
| ATOM | 2220 | O | ASN A 286 | 0.600 | 24.306 | 24.108 | 1.00 | 35.85 | | O |
| ATOM | 2221 | CB | ASN A 286 | -0.336 | 26.635 | 25.274 | 1.00 | 37.80 | | C |
| ATOM | 2222 | CG | ASN A 286 | -0.882 | 27.690 | 26.219 | 1.00 | 42.02 | | C |
| ATOM | 2223 | OD1 | ASN A 286 | -1.326 | 27.365 | 27.326 | 1.00 | 47.86 | | O |
| ATOM | 2224 | ND2 | ASN A 286 | -0.809 | 28.965 | 25.817 | 1.00 | 46.67 | | N |
| ATOM | 2225 | N | GLY A 287 | 2.653 | 24.478 | 24.974 | 1.00 | 35.43 | | N |
| ATOM | 2226 | CA | GLY A 287 | 3.262 | 23.539 | 24.057 | 1.00 | 34.11 | | C |
| ATOM | 2227 | C | GLY A 287 | 3.569 | 22.202 | 24.666 | 1.00 | 34.02 | | C |
| ATOM | 2228 | O | GLY A 287 | 4.073 | 21.317 | 23.977 | 1.00 | 34.98 | | O |
| ATOM | 2229 | N | GLY A 288 | 3.242 | 22.023 | 25.944 | 1.00 | 33.71 | | N |
| ATOM | 2230 | CA | GLY A 288 | 3.476 | 20.759 | 26.616 | 1.00 | 33.00 | | C |
| ATOM | 2231 | C | GLY A 288 | 4.908 | 20.692 | 27.107 | 1.00 | 33.19 | | C |
| ATOM | 2232 | O | GLY A 288 | 5.625 | 21.681 | 26.989 | 1.00 | 33.40 | | O |
| ATOM | 2233 | N | ILE A 289 | 5.337 | 19.540 | 27.621 | 1.00 | 32.87 | | N |
| ATOM | 2234 | CA | ILE A 289 | 6.647 | 19.425 | 28.195 | 1.00 | 33.57 | | C |
| ATOM | 2235 | C | ILE A 289 | 7.695 | 19.434 | 27.118 | 1.00 | 33.13 | | C |
| ATOM | 2236 | O | ILE A 289 | 7.454 | 19.023 | 25.995 | 1.00 | 34.41 | | O |
| ATOM | 2237 | CB | ILE A 289 | 6.809 | 18.137 | 29.006 | 1.00 | 34.25 | | C |
| ATOM | 2238 | CG1 | ILE A 289 | 6.789 | 16.920 | 28.102 | 1.00 | 36.60 | | C |
| ATOM | 2239 | CG2 | ILE A 289 | 5.746 | 18.005 | 30.113 | 1.00 | 34.91 | | C |
| ATOM | 2240 | CD1 | ILE A 289 | 7.271 | 15.659 | 28.834 | 1.00 | 38.16 | | C |
| ATOM | 2241 | N | THR A 290 | 8.891 | 19.868 | 27.465 | 1.00 | 31.68 | | N |
| ATOM | 2242 | CA | THR A 290 | 9.956 | 19.853 | 26.498 | 1.00 | 29.79 | | C |
| ATOM | 2243 | C | THR A 290 | 11.054 | 18.938 | 26.958 | 1.00 | 27.97 | | C |
| ATOM | 2244 | O | THR A 290 | 11.256 | 18.739 | 28.133 | 1.00 | 26.58 | | O |
| ATOM | 2245 | CB | THR A 290 | 10.526 | 21.278 | 26.305 | 1.00 | 30.77 | | C |
| ATOM | 2246 | OG1 | THR A 290 | 10.957 | 21.827 | 27.554 | 1.00 | 27.89 | | O |
| ATOM | 2247 | CG2 | THR A 290 | 9.458 | 22.243 | 25.789 | 1.00 | 30.82 | | C |
| ATOM | 2248 | N | ILE A 291 | 11.787 | 18.395 | 26.021 | 1.00 | 26.96 | | N |
| ATOM | 2249 | CA | ILE A 291 | 12.910 | 17.594 | 26.383 | 1.00 | 27.83 | | C |
| ATOM | 2250 | C | ILE A 291 | 14.059 | 17.952 | 25.493 | 1.00 | 27.31 | | C |
| ATOM | 2251 | O | ILE A 291 | 13.880 | 18.028 | 24.289 | 1.00 | 27.83 | | O |
| ATOM | 2252 | CB | ILE A 291 | 12.596 | 16.104 | 26.195 | 1.00 | 28.72 | | C |
| ATOM | 2253 | CG1 | ILE A 291 | 11.480 | 15.671 | 27.140 | 1.00 | 29.09 | | C |
| ATOM | 2254 | CG2 | ILE A 291 | 13.865 | 15.278 | 26.438 | 1.00 | 28.55 | | C |
| ATOM | 2255 | CD1 | ILE A 291 | 11.115 | 14.232 | 26.986 | 1.00 | 30.86 | | C |
| ATOM | 2256 | N | THR A 292 | 15.240 | 18.093 | 26.074 | 1.00 | 26.63 | | N |
| ATOM | 2257 | CA | THR A 292 | 16.415 | 18.444 | 25.333 | 1.00 | 26.88 | | C |
| ATOM | 2258 | C | THR A 292 | 17.587 | 17.724 | 25.915 | 1.00 | 26.52 | | C |
| ATOM | 2259 | O | THR A 292 | 17.631 | 17.524 | 27.102 | 1.00 | 26.40 | | O |
| ATOM | 2260 | CB | THR A 292 | 16.753 | 19.971 | 25.532 | 1.00 | 27.41 | | C |
| ATOM | 2261 | OG1 | THR A 292 | 15.652 | 20.841 | 25.187 | 1.00 | 28.64 | | O |
| ATOM | 2262 | CG2 | THR A 292 | 17.852 | 20.398 | 24.592 | 1.00 | 28.03 | | C |
| ATOM | 2263 | N | VAL A 293 | 18.577 | 17.414 | 25.093 | 1.00 | 26.32 | | N |
| ATOM | 2264 | CA | VAL A 293 | 19.834 | 16.896 | 25.585 | 1.00 | 26.86 | | C |
| ATOM | 2265 | C | VAL A 293 | 20.964 | 17.718 | 24.978 | 1.00 | 27.24 | | C |
| ATOM | 2266 | O | VAL A 293 | 21.011 | 17.892 | 23.757 | 1.00 | 26.60 | | O |
| ATOM | 2267 | CB | VAL A 293 | 20.029 | 15.422 | 25.226 | 1.00 | 27.56 | | C |
| ATOM | 2268 | CG1 | VAL A 293 | 21.472 | 15.004 | 25.411 | 1.00 | 27.42 | | C |
| ATOM | 2269 | CG2 | VAL A 293 | 19.138 | 14.546 | 26.126 | 1.00 | 29.64 | | C |
| ATOM | 2270 | N | ASN A 294 | 21.849 | 18.278 | 25.814 | 1.00 | 27.26 | | N |
| ATOM | 2271 | CA | ASN A 294 | 22.960 | 19.055 | 25.258 | 1.00 | 27.81 | | C |
| ATOM | 2272 | C | ASN A 294 | 24.253 | 18.268 | 25.281 | 1.00 | 27.79 | | C |
| ATOM | 2273 | O | ASN A 294 | 24.338 | 17.177 | 25.883 | 1.00 | 28.63 | | O |
| ATOM | 2274 | CB | ASN A 294 | 23.118 | 20.446 | 25.881 | 1.00 | 27.69 | | C |
| ATOM | 2275 | CG | ASN A 294 | 23.703 | 20.405 | 27.287 | 1.00 | 30.08 | | C |
| ATOM | 2276 | OD1 | ASN A 294 | 24.309 | 19.397 | 27.677 | 1.00 | 29.80 | | O |
| ATOM | 2277 | ND2 | ASN A 294 | 23.513 | 21.506 | 28.064 | 1.00 | 28.15 | | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2278 | N | PHE | A | 295 | 25.235 | 18.816 | 24.576 | 1.00 | 27.46 | N |
| ATOM | 2279 | CA | PHE | A | 295 | 26.548 | 18.219 | 24.428 | 1.00 | 27.53 | C |
| ATOM | 2280 | C | PHE | A | 295 | 27.543 | 19.352 | 24.675 | 1.00 | 28.01 | C |
| ATOM | 2281 | O | PHE | A | 295 | 27.720 | 20.239 | 23.811 | 1.00 | 28.48 | O |
| ATOM | 2282 | CB | PHE | A | 295 | 26.756 | 17.703 | 23.009 | 1.00 | 27.33 | C |
| ATOM | 2283 | CG | PHE | A | 295 | 25.955 | 16.487 | 22.658 | 1.00 | 27.87 | C |
| ATOM | 2284 | CD1 | PHE | A | 295 | 24.586 | 16.560 | 22.496 | 1.00 | 27.75 | C |
| ATOM | 2285 | CD2 | PHE | A | 295 | 26.581 | 15.287 | 22.426 | 1.00 | 26.57 | C |
| ATOM | 2286 | CE1 | PHE | A | 295 | 23.892 | 15.466 | 22.147 | 1.00 | 28.45 | C |
| ATOM | 2287 | CE2 | PHE | A | 295 | 25.869 | 14.187 | 22.095 | 1.00 | 27.40 | C |
| ATOM | 2288 | CZ | PHE | A | 295 | 24.541 | 14.262 | 21.952 | 1.00 | 27.57 | C |
| ATOM | 2289 | N | TRP | A | 296 | 28.166 | 19.346 | 25.852 | 1.00 | 28.46 | N |
| ATOM | 2290 | CA | TRP | A | 296 | 29.097 | 20.402 | 26.249 | 1.00 | 29.05 | C |
| ATOM | 2291 | C | TRP | A | 296 | 30.545 | 19.950 | 26.077 | 1.00 | 29.39 | C |
| ATOM | 2292 | O | TRP | A | 296 | 30.981 | 18.942 | 26.663 | 1.00 | 29.90 | O |
| ATOM | 2293 | CB | TRP | A | 296 | 28.850 | 20.825 | 27.696 | 1.00 | 29.23 | C |
| ATOM | 2294 | CG | TRP | A | 296 | 27.917 | 21.982 | 27.908 | 1.00 | 31.21 | C |
| ATOM | 2295 | CD1 | TRP | A | 296 | 27.805 | 23.080 | 27.135 | 1.00 | 33.45 | C |
| ATOM | 2296 | CD2 | TRP | A | 296 | 26.995 | 22.171 | 28.996 | 1.00 | 33.70 | C |
| ATOM | 2297 | NE1 | TRP | A | 296 | 26.864 | 23.941 | 27.651 | 1.00 | 33.91 | N |
| ATOM | 2298 | CE2 | TRP | A | 296 | 26.344 | 23.403 | 28.787 | 1.00 | 33.49 | C |
| ATOM | 2299 | CE3 | TRP | A | 296 | 26.638 | 21.414 | 30.113 | 1.00 | 36.30 | C |
| ATOM | 2300 | CZ2 | TRP | A | 296 | 25.377 | 23.902 | 29.642 | 1.00 | 35.59 | C |
| ATOM | 2301 | CZ3 | TRP | A | 296 | 25.643 | 21.899 | 30.967 | 1.00 | 37.80 | C |
| ATOM | 2302 | CH2 | TRP | A | 296 | 25.034 | 23.141 | 30.727 | 1.00 | 37.39 | C |
| ATOM | 2303 | N | TYR | A | 297 | 31.288 | 20.720 | 25.292 | 1.00 | 29.87 | N |
| ATOM | 2304 | CA | TYR | A | 297 | 32.693 | 20.472 | 25.017 | 1.00 | 30.43 | C |
| ATOM | 2305 | C | TYR | A | 297 | 33.548 | 21.629 | 25.518 | 1.00 | 30.98 | C |
| ATOM | 2306 | O | TYR | A | 297 | 33.167 | 22.765 | 25.387 | 1.00 | 29.50 | O |
| ATOM | 2307 | CB | TYR | A | 297 | 32.909 | 20.334 | 23.502 | 1.00 | 30.36 | C |
| ATOM | 2308 | CG | TYR | A | 297 | 32.304 | 19.083 | 22.919 | 1.00 | 30.07 | C |
| ATOM | 2309 | CD1 | TYR | A | 297 | 30.946 | 19.012 | 22.627 | 1.00 | 29.74 | C |
| ATOM | 2310 | CD2 | TYR | A | 297 | 33.083 | 17.960 | 22.687 | 1.00 | 28.56 | C |
| ATOM | 2311 | CE1 | TYR | A | 297 | 30.397 | 17.859 | 22.105 | 1.00 | 28.46 | C |
| ATOM | 2312 | CE2 | TYR | A | 297 | 32.546 | 16.800 | 22.213 | 1.00 | 27.77 | C |
| ATOM | 2313 | CZ | TYR | A | 297 | 31.202 | 16.758 | 21.913 | 1.00 | 28.10 | C |
| ATOM | 2314 | OH | TYR | A | 297 | 30.654 | 15.613 | 21.438 | 1.00 | 27.72 | O |
| ATOM | 2315 | N | LYS | A | 298 | 34.723 | 21.325 | 26.060 | 1.00 | 32.77 | N |
| ATOM | 2316 | CA | LYS | A | 298 | 35.671 | 22.349 | 26.470 | 1.00 | 34.43 | C |
| ATOM | 2317 | C | LYS | A | 298 | 36.126 | 23.014 | 25.216 | 1.00 | 34.91 | C |
| ATOM | 2318 | O | LYS | A | 298 | 36.236 | 22.373 | 24.194 | 1.00 | 35.28 | O |
| ATOM | 2319 | CB | LYS | A | 298 | 36.865 | 21.749 | 27.221 | 1.00 | 35.25 | C |
| ATOM | 2320 | CG | LYS | A | 298 | 36.595 | 21.446 | 28.725 | 1.00 | 38.48 | C |
| ATOM | 2321 | CD | LYS | A | 298 | 37.834 | 20.990 | 29.532 | 1.00 | 42.40 | C |
| ATOM | 2322 | CE | LYS | A | 298 | 37.429 | 20.600 | 30.991 | 1.00 | 45.34 | C |
| ATOM | 2323 | NZ | LYS | A | 298 | 38.515 | 19.883 | 31.770 | 1.00 | 49.07 | N |
| ATOM | 2324 | N | GLY | A | 299 | 36.384 | 24.305 | 25.267 | 1.00 | 36.67 | N |
| ATOM | 2325 | CA | GLY | A | 299 | 36.837 | 24.998 | 24.080 | 1.00 | 38.01 | C |
| ATOM | 2326 | C | GLY | A | 299 | 38.249 | 24.618 | 23.689 | 1.00 | 39.33 | C |
| ATOM | 2327 | O | GLY | A | 299 | 38.965 | 23.987 | 24.437 | 1.00 | 39.19 | O |
| ATOM | 2328 | N | ALA | A | 300 | 38.644 | 25.017 | 22.498 | 1.00 | 41.68 | N |
| ATOM | 2329 | CA | ALA | A | 300 | 40.014 | 24.844 | 22.048 | 1.00 | 43.93 | C |
| ATOM | 2330 | C | ALA | A | 300 | 40.964 | 25.618 | 22.940 | 1.00 | 45.88 | C |
| ATOM | 2331 | O | ALA | A | 300 | 40.558 | 26.437 | 23.741 | 1.00 | 46.12 | O |
| ATOM | 2332 | CB | ALA | A | 300 | 40.148 | 25.343 | 20.639 | 1.00 | 43.86 | C |
| ATOM | 2333 | N | PRO | A | 301 | 42.254 | 25.393 | 22.773 | 1.00 | 49.19 | N |
| ATOM | 2334 | CA | PRO | A | 301 | 43.251 | 26.084 | 23.605 | 1.00 | 50.79 | C |
| ATOM | 2335 | C | PRO | A | 301 | 43.465 | 27.525 | 23.204 | 1.00 | 52.01 | C |
| ATOM | 2336 | O | PRO | A | 301 | 43.302 | 27.869 | 22.041 | 1.00 | 52.73 | O |
| ATOM | 2337 | CB | PRO | A | 301 | 44.534 | 25.325 | 23.303 | 1.00 | 50.51 | C |
| ATOM | 2338 | CG | PRO | A | 301 | 44.357 | 24.908 | 21.884 | 1.00 | 50.75 | C |

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ATOM   2339  CD  PRO A 301      42.890  24.521  21.766  1.00 49.57           C
ATOM   2340  N   THR A 302      43.831  28.346  24.169  1.00 53.76           N
ATOM   2341  CA  THR A 302      44.173  29.736  23.928  1.00 55.20           C
ATOM   2342  C   THR A 302      45.563  29.720  23.307  1.00 56.14           C
ATOM   2343  O   THR A 302      46.504  29.273  23.980  1.00 56.50           O
ATOM   2344  CB  THR A 302      44.249  30.449  25.274  1.00 55.30           C
ATOM   2345  OG1 THR A 302      42.959  30.448  25.909  1.00 57.92           O
ATOM   2346  CG2 THR A 302      44.552  31.886  25.090  1.00 56.33           C
ATOM   2347  N   PRO A 303      45.743  30.239  22.086  1.00 56.60           N
ATOM   2348  CA  PRO A 303      47.057  30.145  21.427  1.00 56.45           C
ATOM   2349  C   PRO A 303      48.168  30.743  22.280  1.00 56.31           C
ATOM   2350  O   PRO A 303      47.845  31.449  23.235  1.00 56.29           O
ATOM   2351  CB  PRO A 303      46.883  30.989  20.168  1.00 56.55           C
ATOM   2352  CG  PRO A 303      45.418  31.007  19.927  1.00 56.34           C
ATOM   2353  CD  PRO A 303      44.812  31.082  21.309  1.00 56.48           C
ATOM   2354  N   GLU A 307      46.896  37.001  18.664  1.00 61.01           N
ATOM   2355  CA  GLU A 307      46.873  37.991  17.591  1.00 61.50           C
ATOM   2356  C   GLU A 307      45.852  39.079  17.834  1.00 60.73           C
ATOM   2357  O   GLU A 307      44.755  38.828  18.308  1.00 61.45           O
ATOM   2358  CB  GLU A 307      46.614  37.356  16.205  1.00 62.21           C
ATOM   2359  CG  GLU A 307      46.871  38.339  15.045  1.00 63.86           C
ATOM   2360  CD  GLU A 307      46.898  37.697  13.665  1.00 65.26           C
ATOM   2361  OE1 GLU A 307      46.468  36.535  13.516  1.00 65.73           O
ATOM   2362  OE2 GLU A 307      47.342  38.382  12.718  1.00 67.94           O
ATOM   2363  N   TYR A 308      46.237  40.302  17.513  1.00 59.88           N
ATOM   2364  CA  TYR A 308      45.349  41.441  17.639  1.00 59.19           C
ATOM   2365  C   TYR A 308      44.706  41.622  16.279  1.00 58.70           C
ATOM   2366  O   TYR A 308      45.224  41.120  15.273  1.00 59.29           O
ATOM   2367  CB  TYR A 308      46.133  42.665  18.095  1.00 59.18           C
ATOM   2368  CG  TYR A 308      46.677  42.418  19.478  1.00 59.73           C
ATOM   2369  CD1 TYR A 308      45.904  42.708  20.605  1.00 59.74           C
ATOM   2370  CD2 TYR A 308      47.912  41.801  19.665  1.00 59.94           C
ATOM   2371  CE1 TYR A 308      46.357  42.438  21.869  1.00 59.94           C
ATOM   2372  CE2 TYR A 308      48.377  41.519  20.933  1.00 61.17           C
ATOM   2373  CZ  TYR A 308      47.592  41.843  22.038  1.00 61.68           C
ATOM   2374  OH  TYR A 308      48.032  41.579  23.316  1.00 63.29           O
ATOM   2375  N   PRO A 309      43.541  42.258  16.233  1.00 57.37           N
ATOM   2376  CA  PRO A 309      42.849  42.815  17.411  1.00 55.72           C
ATOM   2377  C   PRO A 309      42.113  41.742  18.225  1.00 52.85           C
ATOM   2378  O   PRO A 309      41.627  40.815  17.613  1.00 53.22           O
ATOM   2379  CB  PRO A 309      41.823  43.755  16.777  1.00 56.31           C
ATOM   2380  CG  PRO A 309      41.512  43.113  15.410  1.00 57.04           C
ATOM   2381  CD  PRO A 309      42.774  42.431  14.984  1.00 57.43           C
ATOM   2382  N   LEU A 310      41.998  41.879  19.544  1.00 49.67           N
ATOM   2383  CA  LEU A 310      41.368  40.825  20.363  1.00 47.23           C
ATOM   2384  C   LEU A 310      39.870  40.656  20.128  1.00 45.07           C
ATOM   2385  O   LEU A 310      39.131  41.635  19.956  1.00 45.94           O
ATOM   2386  CB  LEU A 310      41.568  41.109  21.837  1.00 46.99           C
ATOM   2387  CG  LEU A 310      42.579  40.351  22.706  1.00 46.52           C
ATOM   2388  CD1 LEU A 310      43.856  40.028  22.048  1.00 45.64           C
ATOM   2389  CD2 LEU A 310      42.840  41.179  23.975  1.00 46.57           C
ATOM   2390  N   LYS A 311      39.408  39.414  20.139  1.00 41.52           N
ATOM   2391  CA  LYS A 311      37.987  39.155  20.003  1.00 38.55           C
ATOM   2392  C   LYS A 311      37.179  39.463  21.276  1.00 35.80           C
ATOM   2393  O   LYS A 311      37.664  39.425  22.400  1.00 34.43           O
ATOM   2394  CB  LYS A 311      37.760  37.727  19.553  1.00 39.46           C
ATOM   2395  N   ALA A 312      35.920  39.786  21.076  1.00 32.82           N
ATOM   2396  CA  ALA A 312      35.055  40.081  22.185  1.00 30.91           C
ATOM   2397  C   ALA A 312      35.152  39.033  23.279  1.00 30.00           C
ATOM   2398  O   ALA A 312      35.231  39.382  24.442  1.00 28.68           O
ATOM   2399  CB  ALA A 312      33.625  40.234  21.707  1.00 30.07           C
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2400 | N | HIS A 313 | 35.148 | 37.753 | 22.916 | 1.00 | 29.85 | N |
| ATOM | 2401 | CA | HIS A 313 | 35.125 | 36.727 | 23.931 | 1.00 | 30.47 | C |
| ATOM | 2402 | C | HIS A 313 | 36.410 | 36.710 | 24.689 | 1.00 | 29.99 | C |
| ATOM | 2403 | O | HIS A 313 | 36.439 | 36.320 | 25.846 | 1.00 | 29.25 | O |
| ATOM | 2404 | CB | HIS A 313 | 34.787 | 35.331 | 23.392 | 1.00 | 31.64 | C |
| ATOM | 2405 | CG | HIS A 313 | 35.860 | 34.714 | 22.566 | 1.00 | 35.54 | C |
| ATOM | 2406 | ND1 | HIS A 313 | 35.987 | 34.950 | 21.208 | 1.00 | 41.10 | N |
| ATOM | 2407 | CD2 | HIS A 313 | 36.844 | 33.846 | 22.891 | 1.00 | 40.77 | C |
| ATOM | 2408 | CE1 | HIS A 313 | 37.047 | 34.303 | 20.750 | 1.00 | 40.02 | C |
| ATOM | 2409 | NE2 | HIS A 313 | 37.567 | 33.603 | 21.743 | 1.00 | 41.82 | N |
| ATOM | 2410 | N | GLN A 314 | 37.482 | 37.137 | 24.056 | 1.00 | 29.68 | N |
| ATOM | 2411 | CA | GLN A 314 | 38.754 | 37.185 | 24.751 | 1.00 | 29.77 | C |
| ATOM | 2412 | C | GLN A 314 | 38.729 | 38.294 | 25.817 | 1.00 | 30.57 | C |
| ATOM | 2413 | O | GLN A 314 | 39.222 | 38.120 | 26.956 | 1.00 | 29.69 | O |
| ATOM | 2414 | CB | GLN A 314 | 39.893 | 37.401 | 23.743 | 1.00 | 30.02 | C |
| ATOM | 2415 | CG | GLN A 314 | 40.111 | 36.182 | 22.786 | 1.00 | 29.84 | C |
| ATOM | 2416 | CD | GLN A 314 | 41.126 | 36.437 | 21.687 | 1.00 | 31.76 | C |
| ATOM | 2417 | OE1 | GLN A 314 | 40.982 | 37.377 | 20.885 | 1.00 | 32.81 | O |
| ATOM | 2418 | NE2 | GLN A 314 | 42.160 | 35.594 | 21.637 | 1.00 | 34.23 | N |
| ATOM | 2419 | N | LYS A 315 | 38.111 | 39.421 | 25.471 | 1.00 | 30.44 | N |
| ATOM | 2420 | CA | LYS A 315 | 38.026 | 40.491 | 26.431 | 1.00 | 31.27 | C |
| ATOM | 2421 | C | LYS A 315 | 37.192 | 40.023 | 27.635 | 1.00 | 30.75 | C |
| ATOM | 2422 | O | LYS A 315 | 37.511 | 40.373 | 28.784 | 1.00 | 29.60 | O |
| ATOM | 2423 | CB | LYS A 315 | 37.461 | 41.752 | 25.808 | 1.00 | 31.76 | C |
| ATOM | 2424 | CG | LYS A 315 | 38.483 | 42.491 | 24.982 | 1.00 | 33.90 | C |
| ATOM | 2425 | CD | LYS A 315 | 37.902 | 43.711 | 24.329 | 1.00 | 37.97 | C |
| ATOM | 2426 | CE | LYS A 315 | 38.911 | 44.380 | 23.419 | 1.00 | 41.69 | C |
| ATOM | 2427 | NZ | LYS A 315 | 38.264 | 45.411 | 22.536 | 1.00 | 44.93 | N |
| ATOM | 2428 | N | VAL A 316 | 36.163 | 39.216 | 27.362 | 1.00 | 29.26 | N |
| ATOM | 2429 | CA | VAL A 316 | 35.318 | 38.731 | 28.422 | 1.00 | 29.23 | C |
| ATOM | 2430 | C | VAL A 316 | 36.152 | 37.841 | 29.339 | 1.00 | 29.87 | C |
| ATOM | 2431 | O | VAL A 316 | 36.075 | 37.926 | 30.584 | 1.00 | 30.33 | O |
| ATOM | 2432 | CB | VAL A 316 | 34.079 | 37.973 | 27.900 | 1.00 | 28.68 | C |
| ATOM | 2433 | CG1 | VAL A 316 | 33.306 | 37.376 | 29.037 | 1.00 | 28.32 | C |
| ATOM | 2434 | CG2 | VAL A 316 | 33.144 | 38.887 | 27.136 | 1.00 | 28.57 | C |
| ATOM | 2435 | N | ALA A 317 | 36.976 | 37.007 | 28.728 | 1.00 | 29.36 | N |
| ATOM | 2436 | CA | ALA A 317 | 37.878 | 36.136 | 29.487 | 1.00 | 29.26 | C |
| ATOM | 2437 | C | ALA A 317 | 38.776 | 36.941 | 30.389 | 1.00 | 28.08 | C |
| ATOM | 2438 | O | ALA A 317 | 39.052 | 36.564 | 31.519 | 1.00 | 27.65 | O |
| ATOM | 2439 | CB | ALA A 317 | 38.733 | 35.267 | 28.561 | 1.00 | 28.70 | C |
| ATOM | 2440 | N | ILE A 318 | 39.211 | 38.068 | 29.873 | 1.00 | 28.33 | N |
| ATOM | 2441 | CA | ILE A 318 | 40.083 | 38.945 | 30.628 | 1.00 | 28.40 | C |
| ATOM | 2442 | C | ILE A 318 | 39.338 | 39.526 | 31.825 | 1.00 | 28.94 | C |
| ATOM | 2443 | O | ILE A 318 | 39.880 | 39.503 | 32.924 | 1.00 | 29.70 | O |
| ATOM | 2444 | CB | ILE A 318 | 40.697 | 40.053 | 29.732 | 1.00 | 27.74 | C |
| ATOM | 2445 | CG1 | ILE A 318 | 41.683 | 39.443 | 28.743 | 1.00 | 28.14 | C |
| ATOM | 2446 | CG2 | ILE A 318 | 41.433 | 41.082 | 30.577 | 1.00 | 27.98 | C |
| ATOM | 2447 | CD1 | ILE A 318 | 42.271 | 40.447 | 27.759 | 1.00 | 29.17 | C |
| ATOM | 2448 | N | MET A 319 | 38.115 | 40.032 | 31.630 | 1.00 | 28.75 | N |
| ATOM | 2449 | CA | MET A 319 | 37.402 | 40.666 | 32.735 | 1.00 | 28.64 | C |
| ATOM | 2450 | C | MET A 319 | 37.140 | 39.669 | 33.877 | 1.00 | 29.22 | C |
| ATOM | 2451 | O | MET A 319 | 37.308 | 39.981 | 35.082 | 1.00 | 30.32 | O |
| ATOM | 2452 | CB | MET A 319 | 36.123 | 41.355 | 32.273 | 1.00 | 28.33 | C |
| ATOM | 2453 | CG | MET A 319 | 36.327 | 42.553 | 31.334 | 1.00 | 27.88 | C |
| ATOM | 2454 | SD | MET A 319 | 34.779 | 43.349 | 30.857 | 1.00 | 29.90 | S |
| ATOM | 2455 | CE | MET A 319 | 34.146 | 42.288 | 29.455 | 1.00 | 28.71 | C |
| ATOM | 2456 | N | ARG A 320 | 36.802 | 38.446 | 33.515 | 1.00 | 29.22 | N |
| ATOM | 2457 | CA | ARG A 320 | 36.543 | 37.429 | 34.520 | 1.00 | 28.75 | C |
| ATOM | 2458 | C | ARG A 320 | 37.806 | 37.221 | 35.325 | 1.00 | 28.81 | C |
| ATOM | 2459 | O | ARG A 320 | 37.782 | 37.132 | 36.569 | 1.00 | 28.76 | O |
| ATOM | 2460 | CB | ARG A 320 | 36.142 | 36.118 | 33.861 | 1.00 | 28.67 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2461 | CG | ARG | A | 320 | 34.810 | 36.125 | 33.120 | 1.00 | 29.62 | C |
| ATOM | 2462 | CD | ARG | A | 320 | 34.371 | 34.747 | 32.603 | 1.00 | 27.74 | C |
| ATOM | 2463 | NE | ARG | A | 320 | 34.193 | 33.843 | 33.716 | 1.00 | 24.81 | N |
| ATOM | 2464 | CZ | ARG | A | 320 | 33.161 | 33.887 | 34.526 | 1.00 | 27.65 | C |
| ATOM | 2465 | NH1 | ARG | A | 320 | 32.180 | 34.752 | 34.330 | 1.00 | 29.97 | N |
| ATOM | 2466 | NH2 | ARG | A | 320 | 33.088 | 33.064 | 35.542 | 1.00 | 27.59 | N |
| ATOM | 2467 | N | ASN | A | 321 | 38.933 | 37.167 | 34.627 | 1.00 | 28.60 | N |
| ATOM | 2468 | CA | ASN | A | 321 | 40.185 | 36.884 | 35.320 | 1.00 | 28.16 | C |
| ATOM | 2469 | C | ASN | A | 321 | 40.526 | 38.003 | 36.291 | 1.00 | 28.13 | C |
| ATOM | 2470 | O | ASN | A | 321 | 40.945 | 37.742 | 37.423 | 1.00 | 29.13 | O |
| ATOM | 2471 | CB | ASN | A | 321 | 41.318 | 36.615 | 34.319 | 1.00 | 28.09 | C |
| ATOM | 2472 | CG | ASN | A | 321 | 41.317 | 35.177 | 33.817 | 1.00 | 27.94 | C |
| ATOM | 2473 | OD1 | ASN | A | 321 | 40.924 | 34.286 | 34.555 | 1.00 | 28.53 | O |
| ATOM | 2474 | ND2 | ASN | A | 321 | 41.751 | 34.946 | 32.560 | 1.00 | 23.58 | N |
| ATOM | 2475 | N | ILE | A | 322 | 40.337 | 39.250 | 35.876 | 1.00 | 27.49 | N |
| ATOM | 2476 | CA | ILE | A | 322 | 40.659 | 40.350 | 36.749 | 1.00 | 27.70 | C |
| ATOM | 2477 | C | ILE | A | 322 | 39.792 | 40.209 | 38.017 | 1.00 | 27.39 | C |
| ATOM | 2478 | O | ILE | A | 322 | 40.284 | 40.315 | 39.101 | 1.00 | 26.48 | O |
| ATOM | 2479 | CB | ILE | A | 322 | 40.353 | 41.680 | 36.059 | 1.00 | 28.04 | C |
| ATOM | 2480 | CG1 | ILE | A | 322 | 41.302 | 41.941 | 34.897 | 1.00 | 30.79 | C |
| ATOM | 2481 | CG2 | ILE | A | 322 | 40.426 | 42.832 | 37.038 | 1.00 | 28.09 | C |
| ATOM | 2482 | CD1 | ILE | A | 322 | 42.756 | 41.766 | 35.226 | 1.00 | 32.31 | C |
| ATOM | 2483 | N | GLU | A | 323 | 38.494 | 39.961 | 37.854 | 1.00 | 27.37 | N |
| ATOM | 2484 | CA | GLU | A | 323 | 37.618 | 39.868 | 38.985 | 1.00 | 27.48 | C |
| ATOM | 2485 | C | GLU | A | 323 | 38.060 | 38.784 | 39.881 | 1.00 | 27.52 | C |
| ATOM | 2486 | O | GLU | A | 323 | 38.096 | 38.956 | 41.079 | 1.00 | 26.90 | O |
| ATOM | 2487 | CB | GLU | A | 323 | 36.183 | 39.637 | 38.558 | 1.00 | 27.48 | C |
| ATOM | 2488 | CG | GLU | A | 323 | 35.592 | 40.849 | 37.910 | 1.00 | 27.65 | C |
| ATOM | 2489 | CD | GLU | A | 323 | 34.199 | 40.631 | 37.318 | 1.00 | 25.69 | C |
| ATOM | 2490 | OE1 | GLU | A | 323 | 33.236 | 40.358 | 38.050 | 1.00 | 24.42 | O |
| ATOM | 2491 | OE2 | GLU | A | 323 | 34.072 | 40.808 | 36.101 | 1.00 | 24.98 | O |
| ATOM | 2492 | N | LYS | A | 324 | 38.419 | 37.659 | 39.297 | 1.00 | 29.13 | N |
| ATOM | 2493 | CA | LYS | A | 324 | 38.845 | 36.508 | 40.097 | 1.00 | 30.35 | C |
| ATOM | 2494 | C | LYS | A | 324 | 40.099 | 36.825 | 40.912 | 1.00 | 31.16 | C |
| ATOM | 2495 | O | LYS | A | 324 | 40.123 | 36.547 | 42.111 | 1.00 | 32.01 | O |
| ATOM | 2496 | CB | LYS | A | 324 | 39.116 | 35.289 | 39.222 | 1.00 | 30.16 | C |
| ATOM | 2497 | CG | LYS | A | 324 | 37.887 | 34.625 | 38.648 | 1.00 | 30.63 | C |
| ATOM | 2498 | CD | LYS | A | 324 | 38.344 | 33.454 | 37.765 | 1.00 | 30.70 | C |
| ATOM | 2499 | CE | LYS | A | 324 | 37.204 | 32.713 | 37.038 | 1.00 | 30.66 | C |
| ATOM | 2500 | NZ | LYS | A | 324 | 37.728 | 31.451 | 36.325 | 1.00 | 27.19 | N |
| ATOM | 2501 | N | MET | A | 325 | 41.119 | 37.401 | 40.270 | 1.00 | 31.84 | N |
| ATOM | 2502 | CA | MET | A | 325 | 42.392 | 37.735 | 40.939 | 1.00 | 32.71 | C |
| ATOM | 2503 | C | MET | A | 325 | 42.216 | 38.743 | 42.078 | 1.00 | 32.44 | C |
| ATOM | 2504 | O | MET | A | 325 | 42.840 | 38.637 | 43.141 | 1.00 | 30.36 | O |
| ATOM | 2505 | CB | MET | A | 325 | 43.417 | 38.276 | 39.923 | 1.00 | 32.98 | C |
| ATOM | 2506 | CG | MET | A | 325 | 43.978 | 37.216 | 39.032 | 1.00 | 36.70 | C |
| ATOM | 2507 | SD | MET | A | 325 | 44.734 | 37.879 | 37.532 | 1.00 | 46.02 | S |
| ATOM | 2508 | CE | MET | A | 325 | 45.616 | 39.197 | 38.250 | 1.00 | 46.11 | C |
| ATOM | 2509 | N | LEU | A | 326 | 41.376 | 39.738 | 41.837 | 1.00 | 33.01 | N |
| ATOM | 2510 | CA | LEU | A | 326 | 41.116 | 40.756 | 42.852 | 1.00 | 34.17 | C |
| ATOM | 2511 | C | LEU | A | 326 | 40.490 | 40.151 | 44.083 | 1.00 | 33.83 | C |
| ATOM | 2512 | O | LEU | A | 326 | 40.871 | 40.464 | 45.188 | 1.00 | 33.22 | O |
| ATOM | 2513 | CB | LEU | A | 326 | 40.185 | 41.818 | 42.305 | 1.00 | 34.61 | C |
| ATOM | 2514 | CG | LEU | A | 326 | 40.740 | 43.194 | 41.974 | 1.00 | 37.32 | C |
| ATOM | 2515 | CD1 | LEU | A | 326 | 42.251 | 43.297 | 41.924 | 1.00 | 39.32 | C |
| ATOM | 2516 | CD2 | LEU | A | 326 | 40.158 | 43.607 | 40.643 | 1.00 | 39.20 | C |
| ATOM | 2517 | N | GLY | A | 327 | 39.534 | 39.262 | 43.861 | 1.00 | 34.50 | N |
| ATOM | 2518 | CA | GLY | A | 327 | 38.842 | 38.569 | 44.930 | 1.00 | 34.87 | C |
| ATOM | 2519 | C | GLY | A | 327 | 39.796 | 37.776 | 45.779 | 1.00 | 35.34 | C |
| ATOM | 2520 | O | GLY | A | 327 | 39.728 | 37.810 | 47.016 | 1.00 | 35.51 | O |
| ATOM | 2521 | N | GLU | A | 328 | 40.725 | 37.081 | 45.139 | 1.00 | 35.88 | N |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2522 | CA | GLU | A | 328 | 41.708 | 36.346 | 45.926 | 1.00 | 36.96 | C |
| ATOM | 2523 | C | GLU | A | 328 | 42.668 | 37.302 | 46.614 | 1.00 | 35.46 | C |
| ATOM | 2524 | O | GLU | A | 328 | 42.958 | 37.144 | 47.799 | 1.00 | 35.65 | O |
| ATOM | 2525 | CB | GLU | A | 328 | 42.465 | 35.340 | 45.074 | 1.00 | 37.89 | C |
| ATOM | 2526 | CG | GLU | A | 328 | 41.555 | 34.272 | 44.481 | 1.00 | 43.40 | C |
| ATOM | 2527 | CD | GLU | A | 328 | 41.694 | 32.905 | 45.135 | 1.00 | 50.39 | C |
| ATOM | 2528 | OE1 | GLU | A | 328 | 42.006 | 32.861 | 46.361 | 1.00 | 53.07 | O |
| ATOM | 2529 | OE2 | GLU | A | 328 | 41.503 | 31.876 | 44.396 | 1.00 | 53.24 | O |
| ATOM | 2530 | N | ALA | A | 329 | 43.110 | 38.331 | 45.906 | 1.00 | 34.23 | N |
| ATOM | 2531 | CA | ALA | A | 329 | 44.130 | 39.208 | 46.469 | 1.00 | 33.82 | C |
| ATOM | 2532 | C | ALA | A | 329 | 43.652 | 40.031 | 47.632 | 1.00 | 33.70 | C |
| ATOM | 2533 | O | ALA | A | 329 | 44.384 | 40.279 | 48.547 | 1.00 | 33.79 | O |
| ATOM | 2534 | CB | ALA | A | 329 | 44.711 | 40.079 | 45.428 | 1.00 | 33.36 | C |
| ATOM | 2535 | N | LEU | A | 330 | 42.410 | 40.451 | 47.602 | 1.00 | 34.57 | N |
| ATOM | 2536 | CA | LEU | A | 330 | 41.869 | 41.243 | 48.694 | 1.00 | 35.04 | C |
| ATOM | 2537 | C | LEU | A | 330 | 41.351 | 40.397 | 49.837 | 1.00 | 35.29 | C |
| ATOM | 2538 | O | LEU | A | 330 | 41.011 | 40.922 | 50.884 | 1.00 | 35.39 | O |
| ATOM | 2539 | CB | LEU | A | 330 | 40.721 | 42.096 | 48.182 | 1.00 | 34.85 | C |
| ATOM | 2540 | CG | LEU | A | 330 | 41.141 | 43.081 | 47.095 | 1.00 | 35.83 | C |
| ATOM | 2541 | CD1 | LEU | A | 330 | 39.907 | 43.564 | 46.304 | 1.00 | 37.05 | C |
| ATOM | 2542 | CD2 | LEU | A | 330 | 41.842 | 44.244 | 47.662 | 1.00 | 34.12 | C |
| ATOM | 2543 | N | GLY | A | 331 | 41.223 | 39.098 | 49.619 | 1.00 | 36.20 | N |
| ATOM | 2544 | CA | GLY | A | 331 | 40.751 | 38.207 | 50.659 | 1.00 | 36.87 | C |
| ATOM | 2545 | C | GLY | A | 331 | 39.260 | 38.250 | 50.957 | 1.00 | 37.48 | C |
| ATOM | 2546 | O | GLY | A | 331 | 38.807 | 37.527 | 51.846 | 1.00 | 38.53 | O |
| ATOM | 2547 | N | ASN | A | 332 | 38.509 | 39.085 | 50.242 | 1.00 | 37.67 | N |
| ATOM | 2548 | CA | ASN | A | 332 | 37.069 | 39.175 | 50.399 | 1.00 | 38.06 | C |
| ATOM | 2549 | C | ASN | A | 332 | 36.446 | 39.652 | 49.088 | 1.00 | 37.75 | C |
| ATOM | 2550 | O | ASN | A | 332 | 36.688 | 40.760 | 48.661 | 1.00 | 37.42 | O |
| ATOM | 2551 | CB | ASN | A | 332 | 36.728 | 40.152 | 51.523 | 1.00 | 38.50 | C |
| ATOM | 2552 | CG | ASN | A | 332 | 35.272 | 40.103 | 51.896 | 1.00 | 40.34 | C |
| ATOM | 2553 | OD1 | ASN | A | 332 | 34.493 | 39.377 | 51.274 | 1.00 | 43.85 | O |
| ATOM | 2554 | ND2 | ASN | A | 332 | 34.894 | 40.841 | 52.937 | 1.00 | 41.75 | N |
| ATOM | 2555 | N | PRO | A | 333 | 35.628 | 38.839 | 48.451 | 1.00 | 37.92 | N |
| ATOM | 2556 | CA | PRO | A | 333 | 35.076 | 39.209 | 47.146 | 1.00 | 37.97 | C |
| ATOM | 2557 | C | PRO | A | 333 | 34.245 | 40.456 | 47.211 | 1.00 | 37.96 | C |
| ATOM | 2558 | O | PRO | A | 333 | 34.086 | 41.143 | 46.204 | 1.00 | 37.81 | O |
| ATOM | 2559 | CB | PRO | A | 333 | 34.182 | 38.024 | 46.770 | 1.00 | 37.85 | C |
| ATOM | 2560 | CG | PRO | A | 333 | 34.327 | 37.037 | 47.801 | 1.00 | 38.26 | C |
| ATOM | 2561 | CD | PRO | A | 333 | 35.161 | 37.530 | 48.908 | 1.00 | 37.98 | C |
| ATOM | 2562 | N | GLN | A | 334 | 33.702 | 40.741 | 48.381 | 1.00 | 38.23 | N |
| ATOM | 2563 | CA | GLN | A | 334 | 32.872 | 41.928 | 48.539 | 1.00 | 38.84 | C |
| ATOM | 2564 | C | GLN | A | 334 | 33.713 | 43.177 | 48.442 | 1.00 | 37.04 | C |
| ATOM | 2565 | O | GLN | A | 334 | 33.185 | 44.254 | 48.276 | 1.00 | 37.42 | O |
| ATOM | 2566 | CB | GLN | A | 334 | 32.041 | 41.870 | 49.850 | 1.00 | 39.97 | C |
| ATOM | 2567 | CG | GLN | A | 334 | 30.696 | 41.057 | 49.612 | 1.00 | 44.72 | C |
| ATOM | 2568 | CD | GLN | A | 334 | 29.669 | 41.117 | 50.756 | 1.00 | 49.62 | C |
| ATOM | 2569 | OE1 | GLN | A | 334 | 29.666 | 42.067 | 51.566 | 1.00 | 53.65 | O |
| ATOM | 2570 | NE2 | GLN | A | 334 | 28.781 | 40.106 | 50.808 | 1.00 | 50.33 | N |
| ATOM | 2571 | N | GLU | A | 335 | 35.026 | 43.036 | 48.489 | 1.00 | 35.15 | N |
| ATOM | 2572 | CA | GLU | A | 335 | 35.872 | 44.193 | 48.385 | 1.00 | 34.55 | C |
| ATOM | 2573 | C | GLU | A | 335 | 36.197 | 44.510 | 46.927 | 1.00 | 33.05 | C |
| ATOM | 2574 | O | GLU | A | 335 | 36.760 | 45.564 | 46.640 | 1.00 | 32.79 | O |
| ATOM | 2575 | CB | GLU | A | 335 | 37.144 | 44.028 | 49.247 | 1.00 | 35.19 | C |
| ATOM | 2576 | CG | GLU | A | 335 | 36.927 | 44.326 | 50.727 | 1.00 | 37.92 | C |
| ATOM | 2577 | CD | GLU | A | 335 | 38.195 | 44.232 | 51.550 | 1.00 | 43.46 | C |
| ATOM | 2578 | OE1 | GLU | A | 335 | 39.179 | 44.916 | 51.179 | 1.00 | 46.92 | O |
| ATOM | 2579 | OE2 | GLU | A | 335 | 38.211 | 43.499 | 52.589 | 1.00 | 49.17 | O |
| ATOM | 2580 | N | VAL | A | 336 | 35.792 | 43.633 | 46.005 | 1.00 | 31.25 | N |
| ATOM | 2581 | CA | VAL | A | 336 | 36.081 | 43.810 | 44.579 | 1.00 | 29.91 | C |
| ATOM | 2582 | C | VAL | A | 336 | 35.505 | 45.076 | 43.957 | 1.00 | 29.08 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2583 | O | VAL | A | 336 | 36.177 | 45.816 | 43.246 | 1.00 | 29.08 | O |
| ATOM | 2584 | CB | VAL | A | 336 | 35.648 | 42.584 | 43.791 | 1.00 | 30.21 | C |
| ATOM | 2585 | CG1 | VAL | A | 336 | 35.743 | 42.805 | 42.325 | 1.00 | 29.11 | C |
| ATOM | 2586 | CG2 | VAL | A | 336 | 36.540 | 41.391 | 44.161 | 1.00 | 29.98 | C |
| ATOM | 2587 | N | GLY | A | 337 | 34.263 | 45.354 | 44.240 | 1.00 | 28.54 | N |
| ATOM | 2588 | CA | GLY | A | 337 | 33.644 | 46.546 | 43.722 | 1.00 | 27.74 | C |
| ATOM | 2589 | C | GLY | A | 337 | 34.285 | 47.848 | 44.130 | 1.00 | 27.24 | C |
| ATOM | 2590 | O | GLY | A | 337 | 34.599 | 48.687 | 43.281 | 1.00 | 26.81 | O |
| ATOM | 2591 | N | PRO | A | 338 | 34.365 | 48.094 | 45.428 | 1.00 | 27.19 | N |
| ATOM | 2592 | CA | PRO | A | 338 | 34.994 | 49.334 | 45.905 | 1.00 | 26.74 | C |
| ATOM | 2593 | C | PRO | A | 338 | 36.378 | 49.553 | 45.328 | 1.00 | 26.42 | C |
| ATOM | 2594 | O | PRO | A | 338 | 36.678 | 50.668 | 44.932 | 1.00 | 27.57 | O |
| ATOM | 2595 | CB | PRO | A | 338 | 35.008 | 49.173 | 47.426 | 1.00 | 25.92 | C |
| ATOM | 2596 | CG | PRO | A | 338 | 33.800 | 48.384 | 47.682 | 1.00 | 27.15 | C |
| ATOM | 2597 | CD | PRO | A | 338 | 33.750 | 47.326 | 46.531 | 1.00 | 27.09 | C |
| ATOM | 2598 | N | LEU | A | 339 | 37.199 | 48.533 | 45.225 | 1.00 | 25.95 | N |
| ATOM | 2599 | CA | LEU | A | 339 | 38.505 | 48.762 | 44.652 | 1.00 | 26.15 | C |
| ATOM | 2600 | C | LEU | A | 339 | 38.384 | 49.205 | 43.192 | 1.00 | 25.74 | C |
| ATOM | 2601 | O | LEU | A | 339 | 39.021 | 50.203 | 42.784 | 1.00 | 23.97 | O |
| ATOM | 2602 | CB | LEU | A | 339 | 39.375 | 47.521 | 44.763 | 1.00 | 27.19 | C |
| ATOM | 2603 | CG | LEU | A | 339 | 40.835 | 47.787 | 44.367 | 1.00 | 28.71 | C |
| ATOM | 2604 | CD1 | LEU | A | 339 | 41.805 | 47.124 | 45.241 | 1.00 | 31.14 | C |
| ATOM | 2605 | CD2 | LEU | A | 339 | 41.028 | 47.264 | 42.987 | 1.00 | 30.12 | C |
| ATOM | 2606 | N | LEU | A | 340 | 37.555 | 48.491 | 42.416 | 1.00 | 25.64 | N |
| ATOM | 2607 | CA | LEU | A | 340 | 37.364 | 48.841 | 40.991 | 1.00 | 25.90 | C |
| ATOM | 2608 | C | LEU | A | 340 | 36.860 | 50.261 | 40.871 | 1.00 | 26.04 | C |
| ATOM | 2609 | O | LEU | A | 340 | 37.324 | 51.044 | 40.034 | 1.00 | 25.93 | O |
| ATOM | 2610 | CB | LEU | A | 340 | 36.399 | 47.900 | 40.293 | 1.00 | 25.64 | C |
| ATOM | 2611 | CG | LEU | A | 340 | 36.996 | 46.521 | 40.072 | 1.00 | 27.50 | C |
| ATOM | 2612 | CD1 | LEU | A | 340 | 35.943 | 45.559 | 39.555 | 1.00 | 26.88 | C |
| ATOM | 2613 | CD2 | LEU | A | 340 | 38.221 | 46.587 | 39.138 | 1.00 | 26.63 | C |
| ATOM | 2614 | N | ASN | A | 341 | 35.914 | 50.610 | 41.720 | 1.00 | 26.45 | N |
| ATOM | 2615 | CA | ASN | A | 341 | 35.377 | 51.963 | 41.669 | 1.00 | 27.35 | C |
| ATOM | 2616 | C | ASN | A | 341 | 36.450 | 52.983 | 41.983 | 1.00 | 27.08 | C |
| ATOM | 2617 | O | ASN | A | 341 | 36.578 | 54.012 | 41.324 | 1.00 | 26.82 | O |
| ATOM | 2618 | CB | ASN | A | 341 | 34.183 | 52.117 | 42.619 | 1.00 | 27.50 | C |
| ATOM | 2619 | CG | ASN | A | 341 | 32.901 | 51.709 | 41.975 | 1.00 | 28.85 | C |
| ATOM | 2620 | OD1 | ASN | A | 341 | 32.509 | 52.283 | 40.957 | 1.00 | 37.23 | O |
| ATOM | 2621 | ND2 | ASN | A | 341 | 32.263 | 50.697 | 42.504 | 1.00 | 29.29 | N |
| ATOM | 2622 | N | THR | A | 342 | 37.234 | 52.665 | 42.994 | 1.00 | 26.89 | N |
| ATOM | 2623 | CA | THR | A | 342 | 38.321 | 53.509 | 43.355 | 1.00 | 27.22 | C |
| ATOM | 2624 | C | THR | A | 342 | 39.301 | 53.629 | 42.191 | 1.00 | 27.16 | C |
| ATOM | 2625 | O | THR | A | 342 | 39.861 | 54.686 | 42.003 | 1.00 | 26.86 | O |
| ATOM | 2626 | CB | THR | A | 342 | 38.995 | 52.934 | 44.568 | 1.00 | 27.76 | C |
| ATOM | 2627 | OG1 | THR | A | 342 | 38.212 | 53.248 | 45.734 | 1.00 | 29.14 | O |
| ATOM | 2628 | CG2 | THR | A | 342 | 40.367 | 53.604 | 44.784 | 1.00 | 28.62 | C |
| ATOM | 2629 | N | MET | A | 343 | 39.502 | 52.560 | 41.419 | 1.00 | 26.80 | N |
| ATOM | 2630 | CA | MET | A | 343 | 40.401 | 52.623 | 40.282 | 1.00 | 27.48 | C |
| ATOM | 2631 | C | MET | A | 343 | 39.927 | 53.552 | 39.174 | 1.00 | 27.78 | C |
| ATOM | 2632 | O | MET | A | 343 | 40.762 | 54.229 | 38.554 | 1.00 | 26.44 | O |
| ATOM | 2633 | CB | MET | A | 343 | 40.602 | 51.253 | 39.634 | 1.00 | 28.13 | C |
| ATOM | 2634 | CG | MET | A | 343 | 41.758 | 50.440 | 40.125 | 1.00 | 30.19 | C |
| ATOM | 2635 | SD | MET | A | 343 | 42.279 | 49.088 | 38.964 | 1.00 | 32.27 | S |
| ATOM | 2636 | CE | MET | A | 343 | 41.049 | 48.127 | 39.221 | 1.00 | 34.83 | C |
| ATOM | 2637 | N | ILE | A | 344 | 38.619 | 53.568 | 38.864 | 1.00 | 28.41 | N |
| ATOM | 2638 | CA | ILE | A | 344 | 38.193 | 54.350 | 37.700 | 1.00 | 29.03 | C |
| ATOM | 2639 | C | ILE | A | 344 | 37.712 | 55.748 | 37.957 | 1.00 | 28.17 | C |
| ATOM | 2640 | O | ILE | A | 344 | 37.879 | 56.587 | 37.064 | 1.00 | 27.26 | O |
| ATOM | 2641 | CB | ILE | A | 344 | 37.146 | 53.650 | 36.818 | 1.00 | 29.47 | C |
| ATOM | 2642 | CG1 | ILE | A | 344 | 35.766 | 53.866 | 37.384 | 1.00 | 32.69 | C |
| ATOM | 2643 | CG2 | ILE | A | 344 | 37.457 | 52.176 | 36.667 | 1.00 | 32.43 | C |

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ATOM   2644  CD1 ILE A 344      34.724  53.358  36.590  1.00 35.46           C
ATOM   2645  N   LYS A 345      37.107  56.032  39.108  1.00 27.79           N
ATOM   2646  CA  LYS A 345      36.518  57.364  39.218  1.00 28.48           C
ATOM   2647  C   LYS A 345      37.489  58.485  39.219  1.00 27.72           C
ATOM   2648  O   LYS A 345      38.428  58.555  40.000  1.00 27.37           O
ATOM   2649  CB  LYS A 345      35.542  57.611  40.343  1.00 29.78           C
ATOM   2650  CG  LYS A 345      35.537  56.758  41.491  1.00 34.49           C
ATOM   2651  CD  LYS A 345      34.075  56.352  41.692  1.00 37.43           C
ATOM   2652  CE  LYS A 345      33.508  57.036  42.904  1.00 40.47           C
ATOM   2653  NZ  LYS A 345      34.223  56.522  44.138  1.00 46.19           N
ATOM   2654  N   GLY A 346      37.218  59.386  38.297  1.00 26.82           N
ATOM   2655  CA  GLY A 346      38.044  60.538  38.108  1.00 25.95           C
ATOM   2656  C   GLY A 346      39.314  60.175  37.392  1.00 25.08           C
ATOM   2657  O   GLY A 346      40.172  61.022  37.244  1.00 24.91           O
ATOM   2658  N   ARG A 347      39.419  58.935  36.944  1.00 24.84           N
ATOM   2659  CA  ARG A 347      40.647  58.436  36.347  1.00 25.30           C
ATOM   2660  C   ARG A 347      40.431  57.848  34.937  1.00 26.05           C
ATOM   2661  O   ARG A 347      41.138  58.196  34.007  1.00 24.59           O
ATOM   2662  CB  ARG A 347      41.279  57.395  37.272  1.00 25.27           C
ATOM   2663  CG  ARG A 347      41.716  57.934  38.696  1.00 24.21           C
ATOM   2664  CD  ARG A 347      43.159  57.506  39.082  1.00 25.10           C
ATOM   2665  NE  ARG A 347      43.175  56.084  39.017  1.00 24.49           N
ATOM   2666  CZ  ARG A 347      44.102  55.293  38.566  1.00 19.51           C
ATOM   2667  NH1 ARG A 347      45.299  55.692  38.195  1.00 21.86           N
ATOM   2668  NH2 ARG A 347      43.802  54.011  38.579  1.00 18.94           N
ATOM   2669  N   TYR A 348      39.438  56.991  34.794  1.00 27.91           N
ATOM   2670  CA  TYR A 348      39.119  56.380  33.507  1.00 29.80           C
ATOM   2671  C   TYR A 348      37.671  56.590  33.065  1.00 32.00           C
ATOM   2672  O   TYR A 348      37.309  56.173  31.964  1.00 32.29           O
ATOM   2673  CB  TYR A 348      39.379  54.877  33.543  1.00 28.38           C
ATOM   2674  CG  TYR A 348      40.836  54.498  33.597  1.00 27.86           C
ATOM   2675  CD1 TYR A 348      41.617  54.473  32.446  1.00 26.79           C
ATOM   2676  CD2 TYR A 348      41.422  54.124  34.787  1.00 25.32           C
ATOM   2677  CE1 TYR A 348      42.945  54.106  32.496  1.00 25.35           C
ATOM   2678  CE2 TYR A 348      42.734  53.762  34.847  1.00 27.07           C
ATOM   2679  CZ  TYR A 348      43.507  53.759  33.700  1.00 26.40           C
ATOM   2680  OH  TYR A 348      44.827  53.378  33.789  1.00 22.93           O
ATOM   2681  N   ASN A 349      36.824  57.193  33.894  1.00 34.78           N
ATOM   2682  CA  ASN A 349      35.426  57.360  33.473  1.00 37.16           C
ATOM   2683  C   ASN A 349      34.997  58.760  33.104  1.00 38.90           C
ATOM   2684  O   ASN A 349      35.690  59.756  33.136  1.00 38.66           O
ATOM   2685  CB  ASN A 349      34.474  56.837  34.493  1.00 36.69           C
ATOM   2686  CG  ASN A 349      34.480  57.633  35.727  1.00 39.34           C
ATOM   2687  OD1 ASN A 349      35.229  58.632  35.875  1.00 40.92           O
ATOM   2688  ND2 ASN A 349      33.654  57.188  36.684  1.00 42.73           N
ATOM   2689  OXT ASN A 349      33.854  58.954  32.689  1.00 44.16           O
TER    2690       ASN A 349
ATOM   2691  N   LEU S 795      45.870  35.442  31.163  1.00 49.68           N
ATOM   2692  CA  LEU S 795      44.790  36.472  31.262  1.00 49.90           C
ATOM   2693  C   LEU S 795      43.668  36.155  30.294  1.00 50.12           C
ATOM   2694  O   LEU S 795      42.492  36.182  30.666  1.00 49.41           O
ATOM   2695  CB  LEU S 795      45.331  37.873  31.004  1.00 50.09           C
ATOM   2696  CG  LEU S 795      44.774  38.924  31.976  1.00 50.19           C
ATOM   2697  CD1 LEU S 795      44.929  38.464  33.388  1.00 50.50           C
ATOM   2698  CD2 LEU S 795      45.436  40.280  31.876  1.00 51.23           C
ATOM   2699  N   THR S 796      44.041  35.979  29.033  1.00 50.69           N
ATOM   2700  CA  THR S 796      43.178  35.421  27.997  1.00 51.67           C
ATOM   2701  C   THR S 796      42.734  33.983  28.241  1.00 51.11           C
ATOM   2702  O   THR S 796      41.884  33.464  27.535  1.00 51.41           O
ATOM   2703  CB  THR S 796      43.888  35.547  26.626  1.00 51.86           C
ATOM   2704  OG1 THR S 796      43.253  34.704  25.671  1.00 56.26           O
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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2705 | CG2 | THR | S | 796 | 45.272 | 34.981 | 26.662 | 1.00 | 52.69 | C |
| ATOM | 2706 | N | SER | S | 797 | 43.261 | 33.330 | 29.248 | 1.00 | 51.51 | N |
| ATOM | 2707 | CA | SER | S | 797 | 42.838 | 31.965 | 29.497 | 1.00 | 52.74 | C |
| ATOM | 2708 | C | SER | S | 797 | 41.471 | 31.865 | 30.165 | 1.00 | 53.39 | C |
| ATOM | 2709 | O | SER | S | 797 | 41.070 | 32.733 | 30.934 | 1.00 | 52.91 | O |
| ATOM | 2710 | CB | SER | S | 797 | 43.850 | 31.247 | 30.351 | 1.00 | 52.86 | C |
| ATOM | 2711 | OG | SER | S | 797 | 43.687 | 31.623 | 31.697 | 1.00 | 55.21 | O |
| ATOM | 2712 | N | TYR | S | 798 | 40.783 | 30.761 | 29.904 | 1.00 | 54.79 | N |
| ATOM | 2713 | CA | TYR | S | 798 | 39.424 | 30.584 | 30.372 | 1.00 | 56.02 | C |
| ATOM | 2714 | C | TYR | S | 798 | 39.168 | 29.271 | 31.042 | 1.00 | 55.81 | C |
| ATOM | 2715 | O | TYR | S | 798 | 39.880 | 28.305 | 30.827 | 1.00 | 56.61 | O |
| ATOM | 2716 | CB | TYR | S | 798 | 38.437 | 30.747 | 29.214 | 1.00 | 56.97 | C |
| ATOM | 2717 | CG | TYR | S | 798 | 38.599 | 29.821 | 28.015 | 1.00 | 60.68 | C |
| ATOM | 2718 | CD1 | TYR | S | 798 | 39.595 | 30.035 | 27.059 | 1.00 | 62.78 | C |
| ATOM | 2719 | CD2 | TYR | S | 798 | 37.689 | 28.783 | 27.793 | 1.00 | 64.68 | C |
| ATOM | 2720 | CE1 | TYR | S | 798 | 39.708 | 29.207 | 25.943 | 1.00 | 65.08 | C |
| ATOM | 2721 | CE2 | TYR | S | 798 | 37.798 | 27.944 | 26.669 | 1.00 | 66.15 | C |
| ATOM | 2722 | CZ | TYR | S | 798 | 38.808 | 28.155 | 25.755 | 1.00 | 65.29 | C |
| ATOM | 2723 | OH | TYR | S | 798 | 38.902 | 27.335 | 24.652 | 1.00 | 64.08 | O |
| ATOM | 2724 | N | ASP | S | 799 | 38.117 | 29.240 | 31.843 | 1.00 | 55.66 | N |
| ATOM | 2725 | CA | ASP | S | 799 | 37.727 | 28.032 | 32.546 | 1.00 | 55.90 | C |
| ATOM | 2726 | C | ASP | S | 799 | 36.636 | 27.385 | 31.739 | 1.00 | 54.64 | C |
| ATOM | 2727 | O | ASP | S | 799 | 36.430 | 27.785 | 30.604 | 1.00 | 55.18 | O |
| ATOM | 2728 | CB | ASP | S | 799 | 37.212 | 28.367 | 33.948 | 1.00 | 56.52 | C |
| ATOM | 2729 | CG | ASP | S | 799 | 37.366 | 27.225 | 34.906 | 1.00 | 57.36 | C |
| ATOM | 2730 | OD1 | ASP | S | 799 | 36.749 | 26.147 | 34.720 | 1.00 | 57.64 | O |
| ATOM | 2731 | OD2 | ASP | S | 799 | 38.108 | 27.331 | 35.881 | 1.00 | 62.28 | O |
| ATOM | 2732 | N | CYS | S | 800 | 35.915 | 26.428 | 32.326 | 1.00 | 53.45 | N |
| ATOM | 2733 | CA | CYS | S | 800 | 34.887 | 25.693 | 31.594 | 1.00 | 52.63 | C |
| ATOM | 2734 | C | CYS | S | 800 | 33.564 | 25.644 | 32.359 | 1.00 | 51.79 | C |
| ATOM | 2735 | O | CYS | S | 800 | 32.871 | 24.632 | 32.357 | 1.00 | 51.30 | O |
| ATOM | 2736 | CB | CYS | S | 800 | 35.372 | 24.282 | 31.327 | 1.00 | 52.47 | C |
| ATOM | 2737 | SG | CYS | S | 800 | 35.703 | 23.408 | 32.872 | 1.00 | 52.72 | S |
| ATOM | 2738 | N | GLU | S | 801 | 33.187 | 26.742 | 32.996 | 1.00 | 50.91 | N |
| ATOM | 2739 | CA | GLU | S | 801 | 31.939 | 26.732 | 33.762 | 1.00 | 50.65 | C |
| ATOM | 2740 | C | GLU | S | 801 | 30.657 | 26.939 | 32.909 | 1.00 | 50.18 | C |
| ATOM | 2741 | O | GLU | S | 801 | 30.617 | 27.687 | 31.928 | 1.00 | 48.39 | O |
| ATOM | 2742 | CB | GLU | S | 801 | 32.008 | 27.713 | 34.929 | 1.00 | 50.49 | C |
| ATOM | 2743 | CG | GLU | S | 801 | 33.199 | 27.450 | 35.853 | 1.00 | 51.78 | C |
| ATOM | 2744 | CD | GLU | S | 801 | 33.234 | 28.359 | 37.092 | 1.00 | 51.24 | C |
| ATOM | 2745 | OE1 | GLU | S | 801 | 32.589 | 28.038 | 38.102 | 1.00 | 49.25 | O |
| ATOM | 2746 | OE2 | GLU | S | 801 | 33.919 | 29.395 | 37.063 | 1.00 | 51.89 | O |
| ATOM | 2747 | N | VAL | S | 802 | 29.624 | 26.213 | 33.320 | 1.00 | 50.54 | N |
| ATOM | 2748 | CA | VAL | S | 802 | 28.338 | 26.161 | 32.650 | 1.00 | 50.71 | C |
| ATOM | 2749 | C | VAL | S | 802 | 27.213 | 26.094 | 33.694 | 1.00 | 51.25 | C |
| ATOM | 2750 | O | VAL | S | 802 | 27.464 | 25.960 | 34.885 | 1.00 | 50.69 | O |
| ATOM | 2751 | CB | VAL | S | 802 | 28.286 | 24.902 | 31.746 | 1.00 | 50.61 | C |
| ATOM | 2752 | CG1 | VAL | S | 802 | 29.420 | 24.932 | 30.727 | 1.00 | 49.62 | C |
| ATOM | 2753 | CG2 | VAL | S | 802 | 28.376 | 23.601 | 32.585 | 1.00 | 49.78 | C |
| ATOM | 2754 | N | ASN | S | 803 | 25.967 | 26.165 | 33.239 | 1.00 | 52.55 | N |
| ATOM | 2755 | CA | ASN | S | 803 | 24.816 | 26.099 | 34.140 | 1.00 | 53.28 | C |
| ATOM | 2756 | C | ASN | S | 803 | 24.516 | 24.663 | 34.561 | 1.00 | 54.95 | C |
| ATOM | 2757 | O | ASN | S | 803 | 23.440 | 24.150 | 34.298 | 1.00 | 54.22 | O |
| ATOM | 2758 | CB | ASN | S | 803 | 23.560 | 26.724 | 33.511 | 1.00 | 53.04 | C |
| ATOM | 2759 | CG | ASN | S | 803 | 23.546 | 28.245 | 33.569 | 1.00 | 51.60 | C |
| ATOM | 2760 | OD1 | ASN | S | 803 | 24.576 | 28.895 | 33.755 | 1.00 | 51.13 | O |
| ATOM | 2761 | ND2 | ASN | S | 803 | 22.367 | 28.817 | 33.406 | 1.00 | 46.28 | N |
| ATOM | 2762 | N | ALA | S | 804 | 25.498 | 24.033 | 35.201 | 1.00 | 57.29 | N |
| ATOM | 2763 | CA | ALA | S | 804 | 25.373 | 22.697 | 35.784 | 1.00 | 59.38 | C |
| ATOM | 2764 | C | ALA | S | 804 | 26.596 | 22.490 | 36.676 | 1.00 | 61.01 | C |
| ATOM | 2765 | O | ALA | S | 804 | 27.667 | 23.026 | 36.407 | 1.00 | 61.45 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2766 | CB | ALA | S | 804 | 25.315 | 21.603 | 34.716 | 1.00 | 59.47 | C |
| ATOM | 2767 | N | PRO | S | 805 | 26.438 | 21.707 | 37.732 | 1.00 | 62.94 | N |
| ATOM | 2768 | CA | PRO | S | 805 | 27.547 | 21.398 | 38.652 | 1.00 | 63.79 | C |
| ATOM | 2769 | C | PRO | S | 805 | 28.616 | 20.498 | 38.003 | 1.00 | 64.48 | C |
| ATOM | 2770 | O | PRO | S | 805 | 28.368 | 19.875 | 36.970 | 1.00 | 65.26 | O |
| ATOM | 2771 | CB | PRO | S | 805 | 26.851 | 20.654 | 39.807 | 1.00 | 63.79 | C |
| ATOM | 2772 | CG | PRO | S | 805 | 25.582 | 20.066 | 39.187 | 1.00 | 63.48 | C |
| ATOM | 2773 | CD | PRO | S | 805 | 25.175 | 21.035 | 38.107 | 1.00 | 63.26 | C |
| ATOM | 2774 | N | ILE | S | 806 | 29.779 | 20.405 | 38.630 | 1.00 | 65.18 | N |
| ATOM | 2775 | CA | ILE | S | 806 | 30.903 | 19.626 | 38.100 | 1.00 | 65.66 | C |
| ATOM | 2776 | C | ILE | S | 806 | 30.853 | 18.145 | 38.489 | 1.00 | 65.84 | C |
| ATOM | 2777 | O | ILE | S | 806 | 30.287 | 17.780 | 39.522 | 1.00 | 66.22 | O |
| ATOM | 2778 | CB | ILE | S | 806 | 32.239 | 20.255 | 38.582 | 1.00 | 65.91 | C |
| ATOM | 2779 | CG1 | ILE | S | 806 | 32.435 | 20.046 | 40.089 | 1.00 | 65.62 | C |
| ATOM | 2780 | CG2 | ILE | S | 806 | 32.267 | 21.765 | 38.255 | 1.00 | 66.46 | C |
| ATOM | 2781 | CD1 | ILE | S | 806 | 33.719 | 20.639 | 40.611 | 1.00 | 65.48 | C |
| ATOM | 2782 | N | LEU | S | 813 | 29.912 | 8.313 | 36.265 | 1.00 | 60.30 | N |
| ATOM | 2783 | CA | LEU | S | 813 | 30.605 | 8.781 | 35.059 | 1.00 | 60.57 | C |
| ATOM | 2784 | C | LEU | S | 813 | 29.707 | 9.617 | 34.157 | 1.00 | 60.31 | C |
| ATOM | 2785 | O | LEU | S | 813 | 28.484 | 9.496 | 34.194 | 1.00 | 60.27 | O |
| ATOM | 2786 | CB | LEU | S | 813 | 31.167 | 7.599 | 34.266 | 1.00 | 60.46 | C |
| ATOM | 2787 | CG | LEU | S | 813 | 32.067 | 6.674 | 35.092 | 1.00 | 60.30 | C |
| ATOM | 2788 | CD1 | LEU | S | 813 | 32.450 | 5.418 | 34.281 | 1.00 | 61.04 | C |
| ATOM | 2789 | CD2 | LEU | S | 813 | 33.301 | 7.421 | 35.602 | 1.00 | 59.11 | C |
| ATOM | 2790 | N | GLN | S | 814 | 30.344 | 10.465 | 33.355 | 1.00 | 60.31 | N |
| ATOM | 2791 | CA | GLN | S | 814 | 29.648 | 11.353 | 32.440 | 1.00 | 60.05 | C |
| ATOM | 2792 | C | GLN | S | 814 | 30.557 | 11.803 | 31.295 | 1.00 | 59.62 | C |
| ATOM | 2793 | O | GLN | S | 814 | 31.765 | 11.584 | 31.322 | 1.00 | 58.97 | O |
| ATOM | 2794 | CB | GLN | S | 814 | 29.176 | 12.583 | 33.194 | 1.00 | 60.41 | C |
| ATOM | 2795 | CG | GLN | S | 814 | 30.302 | 13.488 | 33.634 | 1.00 | 62.13 | C |
| ATOM | 2796 | CD | GLN | S | 814 | 29.826 | 14.603 | 34.559 | 1.00 | 64.43 | C |
| ATOM | 2797 | OE1 | GLN | S | 814 | 29.260 | 14.327 | 35.616 | 1.00 | 65.48 | O |
| ATOM | 2798 | NE2 | GLN | S | 814 | 30.058 | 15.859 | 34.167 | 1.00 | 65.06 | N |
| ATOM | 2799 | N | GLY | S | 815 | 29.960 | 12.456 | 30.302 | 1.00 | 59.55 | N |
| ATOM | 2800 | CA | GLY | S | 815 | 30.675 | 12.927 | 29.136 | 1.00 | 59.21 | C |
| ATOM | 2801 | C | GLY | S | 815 | 31.493 | 11.823 | 28.493 | 1.00 | 59.26 | C |
| ATOM | 2802 | O | GLY | S | 815 | 31.049 | 10.678 | 28.399 | 1.00 | 58.48 | O |
| ATOM | 2803 | N | GLU | S | 816 | 32.693 | 12.183 | 28.049 | 1.00 | 59.73 | N |
| ATOM | 2804 | CA | GLU | S | 816 | 33.604 | 11.254 | 27.392 | 1.00 | 60.76 | C |
| ATOM | 2805 | C | GLU | S | 816 | 33.768 | 9.941 | 28.168 | 1.00 | 61.61 | C |
| ATOM | 2806 | O | GLU | S | 816 | 33.861 | 8.866 | 27.567 | 1.00 | 61.64 | O |
| ATOM | 2807 | CB | GLU | S | 816 | 34.978 | 11.913 | 27.190 | 1.00 | 60.71 | C |
| ATOM | 2808 | CG | GLU | S | 816 | 35.802 | 11.304 | 26.064 | 1.00 | 61.12 | C |
| ATOM | 2809 | CD | GLU | S | 816 | 37.208 | 11.872 | 25.979 | 1.00 | 61.35 | C |
| ATOM | 2810 | OE1 | GLU | S | 816 | 38.066 | 11.370 | 26.730 | 1.00 | 61.67 | O |
| ATOM | 2811 | OE2 | GLU | S | 816 | 37.467 | 12.801 | 25.168 | 1.00 | 60.68 | O |
| ATOM | 2812 | N | GLU | S | 817 | 33.791 | 10.030 | 29.495 | 1.00 | 62.56 | N |
| ATOM | 2813 | CA | GLU | S | 817 | 33.962 | 8.851 | 30.332 | 1.00 | 63.66 | C |
| ATOM | 2814 | C | GLU | S | 817 | 32.748 | 7.929 | 30.260 | 1.00 | 63.92 | C |
| ATOM | 2815 | O | GLU | S | 817 | 32.887 | 6.709 | 30.187 | 1.00 | 63.68 | O |
| ATOM | 2816 | CB | GLU | S | 817 | 34.217 | 9.257 | 31.777 | 1.00 | 63.99 | C |
| ATOM | 2817 | CG | GLU | S | 817 | 35.518 | 10.012 | 31.974 | 1.00 | 65.72 | C |
| ATOM | 2818 | CD | GLU | S | 817 | 35.371 | 11.514 | 31.786 | 1.00 | 69.17 | C |
| ATOM | 2819 | OE1 | GLU | S | 817 | 34.253 | 11.990 | 31.452 | 1.00 | 70.86 | O |
| ATOM | 2820 | OE2 | GLU | S | 817 | 36.384 | 12.228 | 31.984 | 1.00 | 71.76 | O |
| ATOM | 2821 | N | LEU | S | 818 | 31.558 | 8.517 | 30.296 | 1.00 | 64.38 | N |
| ATOM | 2822 | CA | LEU | S | 818 | 30.344 | 7.733 | 30.191 | 1.00 | 65.00 | C |
| ATOM | 2823 | C | LEU | S | 818 | 30.367 | 6.935 | 28.890 | 1.00 | 65.31 | C |
| ATOM | 2824 | O | LEU | S | 818 | 30.166 | 5.723 | 28.901 | 1.00 | 65.41 | O |
| ATOM | 2825 | CB | LEU | S | 818 | 29.092 | 8.624 | 30.232 | 1.00 | 64.90 | C |
| ATOM | 2826 | CG | LEU | S | 818 | 27.770 | 7.844 | 30.163 | 1.00 | 64.94 | C |

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ATOM   2827  CD1 LEU S 818      27.702   6.871  31.316  1.00 66.53           C
ATOM   2828  CD2 LEU S 818      26.551   8.718  30.205  1.00 63.99           C
ATOM   2829  N   LEU S 819      30.647   7.627  27.787  1.00 65.71           N
ATOM   2830  CA  LEU S 819      30.608   7.037  26.445  1.00 66.10           C
ATOM   2831  C   LEU S 819      31.569   5.851  26.294  1.00 66.37           C
ATOM   2832  O   LEU S 819      31.174   4.773  25.852  1.00 65.86           O
ATOM   2833  CB  LEU S 819      30.901   8.122  25.392  1.00 66.04           C
ATOM   2834  CG  LEU S 819      30.860   7.737  23.916  1.00 66.00           C
ATOM   2835  CD1 LEU S 819      29.537   7.149  23.501  1.00 66.14           C
ATOM   2836  CD2 LEU S 819      31.162   8.967  23.083  1.00 67.31           C
ATOM   2837  N   ARG S 820      32.820   6.053  26.684  1.00 66.68           N
ATOM   2838  CA  ARG S 820      33.824   5.013  26.561  1.00 67.34           C
ATOM   2839  C   ARG S 820      33.492   3.801  27.432  1.00 67.41           C
ATOM   2840  O   ARG S 820      33.573   2.643  26.969  1.00 67.19           O
ATOM   2841  CB  ARG S 820      35.196   5.574  26.917  1.00 67.66           C
ATOM   2842  CG  ARG S 820      35.628   6.605  25.907  1.00 69.12           C
ATOM   2843  CD  ARG S 820      37.048   7.061  26.030  1.00 71.00           C
ATOM   2844  NE  ARG S 820      37.309   8.138  25.079  1.00 73.46           N
ATOM   2845  CZ  ARG S 820      38.442   8.839  25.014  1.00 75.31           C
ATOM   2846  NH1 ARG S 820      39.451   8.581  25.851  1.00 75.90           N
ATOM   2847  NH2 ARG S 820      38.566   9.806  24.104  1.00 75.55           N
ATOM   2848  N   ALA S 821      33.118   4.067  28.684  1.00 67.11           N
ATOM   2849  CA  ALA S 821      32.712   2.999  29.580  1.00 66.99           C
ATOM   2850  C   ALA S 821      31.609   2.171  28.898  1.00 66.76           C
ATOM   2851  O   ALA S 821      31.660   0.945  28.889  1.00 66.63           O
ATOM   2852  CB  ALA S 821      32.234   3.562  30.901  1.00 66.88           C
ATOM   2853  N   LEU S 822      30.625   2.851  28.313  1.00 66.58           N
ATOM   2854  CA  LEU S 822      29.538   2.173  27.607  1.00 66.36           C
ATOM   2855  C   LEU S 822      30.027   1.439  26.359  1.00 66.21           C
ATOM   2856  O   LEU S 822      29.429   0.444  25.956  1.00 66.11           O
ATOM   2857  CB  LEU S 822      28.451   3.172  27.223  1.00 66.06           C
ATOM   2858  CG  LEU S 822      27.710   3.789  28.406  1.00 65.45           C
ATOM   2859  CD1 LEU S 822      26.559   4.613  27.885  1.00 65.37           C
ATOM   2860  CD2 LEU S 822      27.213   2.732  29.396  1.00 65.08           C
TER    2861       LEU S 822
HETATM 2862  ZN    ZN A1350      23.324  27.578  28.817  1.00 32.29          ZN
HETATM 2863  C1  OGA A1351      22.262  25.308  27.891  1.00 34.79           C
HETATM 2864  C2  OGA A1351      21.209  25.940  28.487  1.00 32.90           C
HETATM 2865  C4  OGA A1351      18.882  25.730  29.253  1.00 32.24           C
HETATM 2866  C5  OGA A1351      17.543  25.251  28.735  1.00 32.20           C
HETATM 2867  O1  OGA A1351      22.091  24.207  27.399  1.00 33.47           O
HETATM 2868  O2  OGA A1351      23.404  25.817  27.813  1.00 33.83           O
HETATM 2869  O2' OGA A1351      21.299  27.077  29.004  1.00 31.02           O
HETATM 2870  O3  OGA A1351      17.430  24.476  27.795  1.00 33.67           O
HETATM 2871  N1  OGA A1351      20.067  25.271  28.520  1.00 29.83           N
HETATM 2872  O4  OGA A1351      16.551  25.641  29.307  1.00 32.21           O
HETATM 2873  S   SO4 A1352       0.290  25.194  43.827  1.00 90.02           S
HETATM 2874  O1  SO4 A1352       1.120  26.025  44.689  1.00 89.95           O
HETATM 2875  O2  SO4 A1352       1.151  24.261  43.106  1.00 88.91           O
HETATM 2876  O3  SO4 A1352      -0.627  24.447  44.672  1.00 90.38           O
HETATM 2877  O4  SO4 A1352      -0.468  26.028  42.891  1.00 89.30           O
HETATM 2878  S   SO4 A1353       1.893  28.515  29.870  1.00 98.62           S
HETATM 2879  O1  SO4 A1353       3.138  29.102  30.350  1.00 97.69           O
HETATM 2880  O2  SO4 A1353       2.145  27.399  28.947  1.00 97.91           O
HETATM 2881  O3  SO4 A1353       1.205  28.059  31.078  1.00 99.26           O
HETATM 2882  O4  SO4 A1353       1.078  29.515  29.171  1.00 98.46           O
HETATM 2883  O   HOH H   1      38.820  33.858  31.965  1.00 46.43           O
HETATM 2884  O   HOH H   2      33.795  30.509  39.255  1.00 71.93           O
HETATM 2885  O   HOH H   3      34.891  30.536  35.372  1.00 48.26           O
HETATM 2886  O   HOH H   4      35.615  13.844  24.220  1.00 48.67           O
HETATM 2887  O   HOH Z   1      11.592  21.463  13.878  1.00 49.06           O
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HETATM 2888  O   HOH Z   2       9.700  21.662  12.247  1.00 70.56           O
HETATM 2889  O   HOH Z   3       1.136  21.407   7.962  1.00 66.59           O
HETATM 2890  O   HOH Z   4       2.407  19.370   5.351  1.00 60.28           O
HETATM 2891  O   HOH Z   5       1.014  29.292  13.196  1.00 61.25           O
HETATM 2892  O   HOH Z   6       2.256  32.365  14.166  1.00 73.91           O
HETATM 2893  O   HOH Z   7      11.526  44.954  15.330  1.00 68.94           O
HETATM 2894  O   HOH Z   8      -1.438  30.257  22.663  1.00 85.46           O
HETATM 2895  O   HOH Z   9       7.738  30.579  27.736  1.00 46.83           O
HETATM 2896  O   HOH Z  10       3.543  32.597  32.323  1.00 73.21           O
HETATM 2897  O   HOH Z  11       6.618  43.722  26.114  1.00 79.20           O
HETATM 2898  O   HOH Z  12       4.723  37.184  27.600  1.00 69.48           O
HETATM 2899  O   HOH Z  13      10.942  35.610  30.382  1.00 48.93           O
HETATM 2900  O   HOH Z  14      13.888  48.615  19.570  1.00 55.60           O
HETATM 2901  O   HOH Z  15      12.153  41.664  15.818  1.00 61.09           O
HETATM 2902  O   HOH Z  16      15.898  30.602  12.921  1.00 48.84           O
HETATM 2903  O   HOH Z  17      13.629  22.042   7.314  1.00 56.45           O
HETATM 2904  O   HOH Z  18      14.608  26.242  13.702  1.00 55.84           O
HETATM 2905  O   HOH Z  19      21.110  23.978   3.732  1.00 49.91           O
HETATM 2906  O   HOH Z  20      22.517  24.246   0.061  1.00 58.70           O
HETATM 2907  O   HOH Z  21      27.322  30.745   5.813  1.00 71.25           O
HETATM 2908  O   HOH Z  22      26.669  21.831  43.291  1.00 84.79           O
HETATM 2909  O   HOH Z  23      36.928  29.423  21.116  1.00 60.53           O
HETATM 2910  O   HOH Z  24      28.560  37.933  15.396  1.00 65.84           O
HETATM 2911  O   HOH Z  25      29.717  37.018  10.091  1.00 70.57           O
HETATM 2912  O   HOH Z  26      19.889  17.921  13.411  1.00 40.68           O
HETATM 2913  O   HOH Z  27      18.190  15.068  13.047  1.00 45.64           O
HETATM 2914  O   HOH Z  28      19.229  14.479  16.581  1.00 44.23           O
HETATM 2915  O   HOH Z  29       5.509  12.781  28.209  1.00 48.58           O
HETATM 2916  O   HOH Z  30      19.118   6.397  36.829  1.00 62.79           O
HETATM 2917  O   HOH Z  31      33.446  44.026  25.377  1.00 68.72           O
HETATM 2918  O   HOH Z  32       8.427  26.875  44.426  1.00 65.85           O
HETATM 2919  O   HOH Z  33       9.122  31.413  42.815  1.00 79.14           O
HETATM 2920  O   HOH Z  34      15.645  37.855  35.686  1.00 55.81           O
HETATM 2921  O   HOH Z  35      16.264  30.912  40.283  1.00 52.67           O
HETATM 2922  O   HOH Z  36      28.580  24.804  42.231  1.00 71.47           O
HETATM 2923  O   HOH Z  37      25.125  24.702  42.513  1.00 61.76           O
HETATM 2924  O   HOH Z  38      31.710  33.903  46.336  1.00 58.86           O
HETATM 2925  O   HOH Z  39      24.430  38.695  49.842  1.00 64.87           O
HETATM 2926  O   HOH Z  40      21.999  17.349  48.274  1.00 78.90           O
HETATM 2927  O   HOH Z  41      22.174  10.277  34.700  1.00 61.90           O
HETATM 2928  O   HOH Z  42      17.917  -1.798  33.038  1.00 69.51           O
HETATM 2929  O   HOH Z  43      36.654  10.887   7.525  1.00 72.57           O
HETATM 2930  O   HOH Z  44      13.628  20.833  28.536  1.00 46.20           O
HETATM 2931  O   HOH Z  45       3.910  21.434  31.018  1.00 60.17           O
HETATM 2932  O   HOH Z  46      30.778  38.131  33.414  1.00 33.59           O
HETATM 2933  O   HOH Z  47      25.976  26.458  26.213  1.00 38.20           O
HETATM 2934  O   HOH Z  48      35.876  25.491  27.760  1.00 47.36           O
HETATM 2935  O   HOH Z  49      36.704  26.679  21.111  1.00 49.53           O
HETATM 2936  O   HOH Z  50      17.375  16.970  18.001  1.00 37.06           O
HETATM 2937  O   HOH Z  51       5.442  16.762  21.954  1.00 48.45           O
HETATM 2938  O   HOH Z  52       6.786  12.615  22.641  1.00 71.97           O
HETATM 2939  O   HOH Z  53       7.201  17.017  20.359  1.00 48.19           O
HETATM 2940  O   HOH Z  54       6.512  22.748  23.330  1.00 52.43           O
HETATM 2941  O   HOH Z  55      29.528  38.794  26.547  1.00 33.74           O
HETATM 2942  O   HOH Z  56      30.683  39.271  19.412  1.00 42.04           O
HETATM 2943  O   HOH Z  57      26.571  42.213  18.009  1.00 59.45           O
HETATM 2944  O   HOH Z  58      29.038  40.259  16.007  1.00 65.33           O
HETATM 2945  O   HOH Z  59      27.631  44.557  31.407  1.00 36.71           O
HETATM 2946  O   HOH Z  60      27.654  48.738  30.067  1.00 46.82           O
HETATM 2947  O   HOH Z  61      30.426  45.052  25.424  1.00 49.55           O
HETATM 2948  O   HOH Z  62      25.946  50.745  30.903  1.00 51.76           O
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HETATM 2949  O   HOH Z  63      26.759  31.212  38.332  1.00 39.21           O
HETATM 2950  O   HOH Z  64      29.563  36.988  35.538  1.00 36.58           O
HETATM 2951  O   HOH Z  65      30.608  30.268  36.508  1.00 39.97           O
HETATM 2952  O   HOH Z  66      19.823  31.620  33.966  1.00 44.64           O
HETATM 2953  O   HOH Z  67      19.517  36.182  33.531  1.00 39.38           O
HETATM 2954  O   HOH Z  68      18.255  38.678  36.813  1.00 57.99           O
HETATM 2955  O   HOH Z  69      21.026  42.838  40.240  1.00 56.11           O
HETATM 2956  O   HOH Z  70      17.610  37.832  32.310  1.00 47.08           O
HETATM 2957  O   HOH Z  71      15.109  37.973  32.827  1.00 45.82           O
HETATM 2958  O   HOH Z  72      16.418  47.375  39.219  1.00 67.81           O
HETATM 2959  O   HOH Z  73      15.605  44.895  35.040  1.00 43.78           O
HETATM 2960  O   HOH Z  74      15.286  55.715  27.660  1.00 67.46           O
HETATM 2961  O   HOH Z  75      15.476  50.403  22.363  1.00 44.42           O
HETATM 2962  O   HOH Z  76      16.645  46.682  22.198  1.00 39.25           O
HETATM 2963  O   HOH Z  77      26.589  40.795  15.622  1.00 68.21           O
HETATM 2964  O   HOH Z  78      10.674  19.290  14.058  1.00 55.87           O
HETATM 2965  O   HOH Z  79      27.773  27.556  24.476  1.00 37.12           O
HETATM 2966  O   HOH Z  80      30.214  36.062  27.011  1.00 40.11           O
HETATM 2967  O   HOH Z  81      32.661  34.179  19.369  1.00 54.04           O
HETATM 2968  O   HOH Z  82      27.339  30.221  25.948  1.00 38.07           O
HETATM 2969  O   HOH Z  83      16.261  36.239  29.815  1.00 43.65           O
HETATM 2970  O   HOH Z  84       6.400  23.973  25.697  1.00 45.37           O
HETATM 2971  O   HOH Z  85       4.061  20.777  20.758  1.00 74.60           O
HETATM 2972  O   HOH Z  86      42.841  37.277  18.598  1.00 67.00           O
HETATM 2973  O   HOH Z  87      42.456  44.259  19.547  1.00 64.85           O
HETATM 2974  O   HOH Z  88      33.750  36.936  20.231  1.00 46.70           O
HETATM 2975  O   HOH Z  89      33.208  39.305  33.829  1.00 37.00           O
HETATM 2976  O   HOH Z  90      32.098  40.251  44.432  1.00 46.81           O
HETATM 2977  O   HOH Z  91      32.904  43.762  45.581  1.00 58.90           O
HETATM 2978  O   HOH Z  92      39.242  57.294  42.204  1.00 36.08           O
HETATM 2979  O   HOH Z  93      46.926  53.378  32.000  1.00 42.91           O
HETATM 2980  O   HOH Z  94      37.922  55.476  29.664  1.00 46.42           O
HETATM 2981  O   HOH Z  95      38.489  59.800  33.014  1.00 55.47           O
CONECT 1478 2862
CONECT 1498 2862
CONECT 2167 2862
CONECT 2862 2869 2868 1478 2167 1498
CONECT 2863 2864 2867 2868
CONECT 2864 2863 2869 2871
CONECT 2865 2866 2871
CONECT 2866 2865 2870 2872
CONECT 2867 2863
CONECT 2868 2863 2862
CONECT 2869 2864 2862
CONECT 2870 2866
CONECT 2871 2864 2865
CONECT 2872 2866
CONECT 2873 2874 2875 2876 2877
CONECT 2874 2873
CONECT 2875 2873
CONECT 2876 2873
CONECT 2877 2873
CONECT 2878 2879 2880 2881 2882
CONECT 2879 2878
CONECT 2880 2878
CONECT 2881 2878
CONECT 2882 2878
MASTER      446    0    4   15   20    0    8    6 2979    2   24   31
END
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Structure 4

Below are the coordinates for structure 4 (the 2.85 Å structure of FIH:Fe(II):2OG):

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HEADER    TRANSCRIPTION ACTIVATOR/INHIBITOR       12-AUG-02   1H2N
TITLE     FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX WITH HIF-1 ALPHA
TITLE    2 FRAGMENT PEPTIDE
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: FACTOR INHIBITING HIF1;
COMPND   3 SYNONYM: FIH1;
COMPND   4 CHAIN: A;
COMPND   5 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE   3 ORGANISM_COMMON: HUMAN;
SOURCE   4 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE   5 EXPRESSION_SYSTEM_STRAIN: BL21(DE3);
SOURCE   6 EXPRESSION_SYSTEM_PLASMID: PET28A(+)
KEYWDS    FIH, HIF, DSBH, OXYGENASE, TRANSCRIPTION, HYPOXIA,
KEYWDS   2 2-OXOGLUTARATE, ASPARAGINYL HYDROXYLASE, HYDROXYLASE
EXPDTA    X-RAY DIFFRACTION
AUTHOR    J.M.ELKINS,K.S.HEWITSON,L.A.MCNEILL,I.SCHLEMMINGER,
AUTHOR   2 J.F.SEIBEL,C.J.SCHOFIELD
REVDAT   1   04-SEP-02 1H2N    0
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JRNL        AUTH 2 I.SCHLEMMINGER,J.F.SEIBEL,C.J.SCHOFIELD
JRNL        TITL   FIH:HIF-FRAGMENT COMPLEXES
JRNL        REF    TO BE PUBLISHED
JRNL        REFN
REMARK   2
REMARK   2 RESOLUTION. 2.84 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.0
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) :   2.84
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) :  30.00
REMARK   3   DATA CUTOFF            (SIGMA(F)) : NONE
REMARK   3   COMPLETENESS FOR RANGE        (%) :  99.51
REMARK   3   NUMBER OF REFLECTIONS             :   12577
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD           : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION   : RANDOM
REMARK   3   R VALUE     (WORKING + TEST SET) : 0.23287
REMARK   3   R VALUE           (WORKING SET) :  0.23094
REMARK   3   FREE R VALUE                     :  0.25695
REMARK   3   FREE R VALUE TEST SET SIZE   (%) :  7.7
REMARK   3   FREE R VALUE TEST SET COUNT      :  1046
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           :      20
REMARK   3   BIN RESOLUTION RANGE HIGH           :   2.840
REMARK   3   BIN RESOLUTION RANGE LOW            :   2.913
REMARK   3   REFLECTION IN BIN     (WORKING SET) :     828
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REMARK   3   BIN R VALUE           (WORKING SET) :    0.286
REMARK   3   BIN FREE R VALUE SET COUNT          :      81
REMARK   3   BIN FREE R VALUE                    :    0.315
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 2689
REMARK   3   NUCLEIC ACID ATOMS       : 0
REMARK   3   HETEROGEN ATOMS          : 26
REMARK   3   SOLVENT ATOMS            : 3
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) :  35.345
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :    -1.02
REMARK   3    B22 (A**2) :    -1.02
REMARK   3    B33 (A**2) :     2.03
REMARK   3    B12 (A**2) :     0.00
REMARK   3    B13 (A**2) :     0.00
REMARK   3    B23 (A**2) :     0.00
REMARK   3
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                                (A):   0.852
REMARK   3   ESU BASED ON FREE R VALUE                           (A):   0.349
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                     (A):   0.398
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):  19.679
REMARK   3
REMARK   3 CORRELATION COEFFICIENTS.
REMARK   3   CORRELATION COEFFICIENT FO-FC      :   0.913
REMARK   3   CORRELATION COEFFICIENT FO-FC FREE :   0.901
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES         COUNT    RMS     WEIGHT
REMARK   3   BOND LENGTHS REFINED ATOMS        (A):  2791 ; 0.015 ; 0.021
REMARK   3   BOND LENGTHS OTHERS               (A):  2388 ; 0.001 ; 0.020
REMARK   3   BOND ANGLES REFINED ATOMS   (DEGREES):  3799 ; 1.628 ; 1.945
REMARK   3   BOND ANGLES OTHERS          (DEGREES):  5576 ; 0.823 ; 3.000
REMARK   3   TORSION ANGLES, PERIOD 1    (DEGREES):   330 ; 4.268 ; 3.000
REMARK   3   TORSION ANGLES, PERIOD 3    (DEGREES):   479 ;18.082 ;15.000
REMARK   3   CHIRAL-CENTER RESTRAINTS      (A**3):   384 ; 0.095 ; 0.200
REMARK   3   GENERAL PLANES REFINED ATOMS      (A):  3137 ; 0.005 ; 0.020
REMARK   3   GENERAL PLANES OTHERS             (A):   575 ; 0.002 ; 0.020
REMARK   3   NON-BONDED CONTACTS REFINED ATOMS (A):   717 ; 0.255 ; 0.300
REMARK   3   NON-BONDED CONTACTS OTHERS        (A):  2425 ; 0.224 ; 0.300
REMARK   3   H-BOND (X...Y) REFINED ATOMS      (A):   165 ; 0.139 ; 0.500
REMARK   3   H-BOND (X...Y) OTHERS             (A):     1 ; 0.102 ; 0.500
REMARK   3   POTENTIAL METAL-ION REFINED ATOMS (A):     3 ; 0.112 ; 0.500
REMARK   3   SYMMETRY VDW REFINED ATOMS        (A):    14 ; 0.256 ; 0.300
REMARK   3   SYMMETRY VDW OTHERS               (A):    62 ; 0.273 ; 0.300
REMARK   3   SYMMETRY H-BOND REFINED ATOMS     (A):     4 ; 0.214 ; 0.500
REMARK   3   SYMMETRY H-BOND OTHERS            (A):     1 ; 0.061 ; 0.500
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     COUNT    RMS     WEIGHT
REMARK   3   MAIN-CHAIN BOND REFINED ATOMS (A**2):  1659 ; 0.312 ; 1.500
REMARK   3   MAIN-CHAIN ANGLE REFINED ATOMS (A**2):  2675 ; 0.598 ; 2.000
REMARK   3   SIDE-CHAIN BOND REFINED ATOMS (A**2):  1132 ; 1.058 ; 3.000
REMARK   3   SIDE-CHAIN ANGLE REFINED ATOMS (A**2):  1124 ; 1.795 ; 4.500
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF NCS GROUPS : NULL
REMARK   3
REMARK   3  TLS DETAILS
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REMARK   3   NUMBER OF TLS GROUPS  :    1
REMARK   3
REMARK   3   TLS GROUP :      1
REMARK   3    NUMBER OF COMPONENTS GROUP :    1
REMARK   3    COMPONENTS        C SSSEQI   TO  C SSSEQI
REMARK   3    RESIDUE RANGE :   A    15        A   452
REMARK   3    ORIGIN FOR THE GROUP (A):  21.4490  27.4200  27.7870
REMARK   3    T TENSOR
REMARK   3      T11:   0.2230 T22:   0.0562
REMARK   3      T33:   0.0967 T12:   0.0111
REMARK   3      T13:  -0.0923 T23:   0.0525
REMARK   3    L TENSOR
REMARK   3      L11:   1.6842 L22:   4.4489
REMARK   3      L33:   2.0658 L12:   1.5597
REMARK   3      L13:   1.1572 L23:   2.3523
REMARK   3    S TENSOR
REMARK   3      S11:   0.1098 S12:  -0.2106 S13:  -0.0766
REMARK   3      S21:   0.3449 S22:  -0.0455 S23:   0.2455
REMARK   3      S31:   0.3515 S32:  -0.1199 S33:  -0.0643
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED : BABINET MODEL WITH MASK
REMARK   3   PARAMETERS FOR MASK CALCULATION
REMARK   3   VDW PROBE RADIUS    :   1.40
REMARK   3   ION PROBE RADIUS    :   0.80
REMARK   3   SHRINKAGE RADIUS    :   0.80
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: SEE REMARK 400
REMARK   4
REMARK   4 1H2N COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY EBI  ON 12-AUG-2002.
REMARK 100 THE EBI ID CODE IS EBI-11174.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : 15-MAY-2002
REMARK 200  TEMPERATURE           (KELVIN) : 100
REMARK 200  PH                             : 7.5
REMARK 200  NUMBER OF CRYSTALS USED        : 1
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : Y
REMARK 200  RADIATION SOURCE               : SRS BEAMLINE PX9.5
REMARK 200  BEAMLINE                       : PX9.5
REMARK 200  X-RAY GENERATOR MODEL          : NULL
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M
REMARK 200  WAVELENGTH OR RANGE        (A) : 0.92
REMARK 200  MONOCHROMATOR                  : NULL
REMARK 200  OPTICS                         : NULL
REMARK 200
REMARK 200  DETECTOR TYPE                  : MARCCD
REMARK 200  DETECTOR MANUFACTURER          : MARRESEARCH
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : MOSFLM
REMARK 200  DATA SCALING SOFTWARE          : SCALA
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 13703
REMARK 200  RESOLUTION RANGE HIGH      (A) : 2.84
REMARK 200  RESOLUTION RANGE LOW       (A) : 34.1
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : NONE
REMARK 200
REMARK 200 OVERALL.
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REMARK 200  COMPLETENESS FOR RANGE      (%) : 99.2
REMARK 200  DATA REDUNDANCY                 : 6.7
REMARK 200  R MERGE                     (I) : 0.067
REMARK 200  R SYM                       (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET   : 9.4
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.84
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.99
REMARK 200  COMPLETENESS FOR SHELL      (%) : 94.9
REMARK 200  DATA REDUNDANCY IN SHELL        : 5.2
REMARK 200  R MERGE FOR SHELL           (I) : 0.309
REMARK 200  R SYM FOR SHELL             (I) : NULL
REMARK 200  <I/SIGMA(I)> FOR SHELL          : 2.4
REMARK 200
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT
REMARK 200 SOFTWARE USED: NULL
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: SEE REMARK 400
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 63
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 3.4
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: 1.2M AMMONIUM SULPHATE,
REMARK 280  4% PEG400, 0.1M HEPES PH7.5 ARGON ATMOSPHERE,
REMARK 280  11MG/ML PROTEIN WITH 1MM FE(II), 2.5MM AKG AND 2.5MM
REMARK 280  PEPTIDE (SEE REMARK 400)
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 41 21 2
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
REMARK 290       2555   -X,-Y,1/2+Z
REMARK 290       3555   1/2-Y,1/2+X,1/4+Z
REMARK 290       4555   1/2+Y,1/2-X,3/4+Z
REMARK 290       5555   1/2-X,1/2+Y,1/4-Z
REMARK 290       6555   1/2+X,1/2-Y,3/4-Z
REMARK 290       7555   Y,X,-Z
REMARK 290       8555   -Y,-X,1/2-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   2  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000       73.36600
REMARK 290   SMTRY1   3  0.000000 -1.000000  0.000000       43.17100
REMARK 290   SMTRY2   3  1.000000  0.000000  0.000000       43.17100
REMARK 290   SMTRY3   3  0.000000  0.000000  1.000000       36.68300
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REMARK 290    SMTRY1    4  0.000000  1.000000  0.000000        43.17100
REMARK 290    SMTRY2    4 -1.000000  0.000000  0.000000        43.17100
REMARK 290    SMTRY3    4  0.000000  0.000000  1.000000       110.04900
REMARK 290    SMTRY1    5 -1.000000  0.000000  0.000000        43.17100
REMARK 290    SMTRY2    5  0.000000  1.000000  0.000000        43.17100
REMARK 290    SMTRY3    5  0.000000  0.000000 -1.000000        36.68300
REMARK 290    SMTRY1    6  1.000000  0.000000  0.000000        43.17100
REMARK 290    SMTRY2    6  0.000000 -1.000000  0.000000        43.17100
REMARK 290    SMTRY3    6  0.000000  0.000000 -1.000000       110.04900
REMARK 290    SMTRY1    7  0.000000  1.000000  0.000000         0.00000
REMARK 290    SMTRY2    7  1.000000  0.000000  0.000000         0.00000
REMARK 290    SMTRY3    7  0.000000  0.000000 -1.000000         0.00000
REMARK 290    SMTRY1    8  0.000000 -1.000000  0.000000         0.00000
REMARK 290    SMTRY2    8 -1.000000  0.000000  0.000000         0.00000
REMARK 290    SMTRY3    8  0.000000  0.000000 -1.000000        73.36600
REMARK 290
REMARK 290 REMARK: NULL
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT
REMARK 300 WHICH CONSISTS OF   2 CHAIN(S). SEE REMARK 350 FOR
REMARK 300 INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).
REMARK 300
REMARK 300 QUATERNARY STRUCTURE FOR THIS ENTRY: DIMERIC
REMARK 300
REMARK 300 THE PROTEIN IS A HOMODIMER FORMED BY CHAIN A.
REMARK 300
REMARK 300 FOR THE HOMO-ASSEMBLY DESCRIBED BY REMARK 350
REMARK 300 THE DIFFERENCE IN ACCESSIBLE SURFACE AREA PER
REMARK 300 CHAIN BETWEEN THE ISOLATED CHAIN AND THAT FOR
REMARK 300 THE CHAIN IN THE COMPLEX IS  1600.4 ANGSTROM**2
REMARK 350
REMARK 350 GENERATING THE BIOMOLECULE
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW.  BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE:  1
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A
REMARK 350   BIOMT1   1  1.000000  0.000000  0.000000         0.00000
REMARK 350   BIOMT2   1  0.000000  1.000000  0.000000         0.00000
REMARK 350   BIOMT3   1  0.000000  0.000000  1.000000         0.00000
REMARK 350   BIOMT1   2  0.000000 -1.000000  0.000000        86.34200
REMARK 350   BIOMT2   2 -1.000000  0.000000  0.000000        86.34200
REMARK 350   BIOMT3   2  0.000000  0.000000 -1.000000        73.36600
REMARK 400
REMARK 400 COMPOUND
REMARK 400
REMARK 400  THE PROTEIN (CHAIN A) WAS CRYSTALLIZED IN THE PRESENCE
REMARK 400  OF A PEPTIDE FRAGEMENT FROM ENDOTHELIAL PAS DOMAIN PROTEIN 1
REMARK 400  SWISS-PROT ID Q99814 (RESIDUES 846-858) BUT NONE OF THE
REMARK 400  RESIDUES CORRESPONDING TO THE PEPTIDE WERE VISIBLE IN THE
REMARK 400  ELECTRON DENSITY MAPS. IT IS POSSIBLE THAT THE PEPTIDE DID
REMARK 400  NOT BIND TO THE PROTEIN AND HENCE HAS NOT BEEN INCLUDED IN THE
REMARK 400  COMPND, SOURCE AND SEQRES RECORDS.
REMARK 400
REMARK 400  THE SEQUENCE OF THE FRAGMENT IS GIVEN BELOW.
REMARK 400
REMARK 400  VAL ASN VAL PRO VAL LEU GLY SER SER THR LEU LEU GLN
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REMARK 465
REMARK 465 MISSING RESIDUES
REMARK 465 THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE
REMARK 465 EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 465 IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)
REMARK 465
REMARK 465   M RES C SSSEQI
REMARK 465     MET A     1
REMARK 465     ALA A     2
REMARK 465     ALA A     3
REMARK 465     THR A     4
REMARK 465     ALA A     5
REMARK 465     ALA A     6
REMARK 465     GLU A     7
REMARK 465     ALA A     8
REMARK 465     VAL A     9
REMARK 465     ALA A    10
REMARK 465     SER A    11
REMARK 465     GLY A    12
REMARK 465     SER A    13
REMARK 465     GLY A    14
REMARK 465     LYS A   304
REMARK 465     ARG A   305
REMARK 465     ILE A   306
REMARK 470
REMARK 470 MISSING ATOM
REMARK 470 THE FOLLOWING RESIDUES HAVE MISSING ATOMS (M=MODEL NUMBER;
REMARK 470 RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE NUMBER;
REMARK 470 I=INSERTION CODE):
REMARK 470   M RES CSSEQI  ATOMS
REMARK 470     GLU A  15    CG   CD   OE1  OE2
REMARK 470     GLU A  29    CG   CD   OE1  OE2
REMARK 470     ASN A  87    CG   OD1  ND2
REMARK 470     LYS A 106    CD   CE   NZ
REMARK 470     LYS A 115    CG   CD   CE   NZ
REMARK 470     ARG A 117    CG   CD   NE   CZ   NH1  NH2
REMARK 470     GLN A 133    CG   CD   OE1  NE2
REMARK 470     GLN A 136    CG   CD   OE1  NE2
REMARK 470     GLN A 137    CG   CD   OE1  NE2
REMARK 470     ARG A 156    CG   CD   NE   CZ   NH1  NH2
REMARK 470     LYS A 157    CD   CE   NZ
REMARK 470     LYS A 311    CG   CD   CE   NZ
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND ANGLES
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN
REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)
REMARK 500
REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1   ATM2   ATM3
REMARK 500    TYR A 261   N    -  CA  -  C   ANGL. DEV. = -10.1 DEGREES
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
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REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: COVALENT BOND LENGTHS
REMARK 500
REMARK 500 THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES
REMARK 500 HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE
REMARK 500 THAN 6*RMSD AND BY MORE THAN 0.150 ANGSTROMS (M=MODEL
REMARK 500 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 500 NUMBER; I=INSERTION CODE).
REMARK 500
REMARK 500 STANDARD TABLE:
REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,1X,2(A4,A1,3X),12X,F5.3)
REMARK 500
REMARK 500 EXPECTED VALUESS: ENGH AND HUBER, 1991
REMARK 500
REMARK 500  M RES CSSEQI ATM1   RES CSSEQI ATM2   DEVIATION
REMARK 500    MET A 343  SD     MET A 343  CE      -0.151
REMARK 500
REMARK 500 REMARK: NULL
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500  ATM1  RES C  SSEQI   ATM2  RES C  SSEQI          DISTANCE
REMARK 500
REMARK 500   OG1  THR A    39     OE1  GLU A   262              2.16
REMARK 525
REMARK 525 SOLVENT
REMARK 525
REMARK 525 THE SOLVENT MOLECULES ARE GIVEN CHAIN IDENTIFIERS TO
REMARK 525 INDICATE THE PROTEIN CHAIN TO WHICH THEY ARE MOST CLOSELY
REMARK 525 ASSOCIATED WITH:
REMARK 525   PROTEIN CHAIN  SOLVENT CHAIN
REMARK 525     A              Z
REMARK 600
REMARK 600 HETEROGEN
REMARK 600
REMARK 600 FOR METAL ATOM FE   FE2 A1350  THE COORDINATION ANGLES ARE:
REMARK 600  1 HIS   199A  NE2
REMARK 600  2 ASP   201A  OD2       106.1
REMARK 600  3 HIS   279A  NE2        77.8  85.5
REMARK 600  4 AKG  1351A  O1        168.0  81.1  93.4
REMARK 600  5 AKG  1351A  O5         88.7 163.3  90.2  83.1
REMARK 600                            1     2     3     4
REMARK 700
REMARK 700 SHEET
REMARK 700 THE SHEET STRUCTURE OF THIS MOLECULE IS BIFURCATED. IN
REMARK 700 ORDER TO REPRESENT THIS FEATURE IN THE SHEET RECORDS BELOW,
REMARK 700 TWO SHEETS ARE DEFINED.
REMARK 800
REMARK 800 SITE
REMARK 800 SITE_IDENTIFIER: FEA
REMARK 800 SITE_DESCRIPTION: FE BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: AKG
REMARK 800 SITE_DESCRIPTION: AKG BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: SA1
REMARK 800 SITE_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
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REMARK 800 SITE_IDENTIFIER: SA2
REMARK 800 SITE_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 800
REMARK 800 SITE_IDENTIFIER: SA3
REMARK 800 SITE_DESCRIPTION: SO4 BINDING SITE FOR CHAIN A
REMARK 900
REMARK 900 RELATED ENTRIES
REMARK 900 RELATED ID: 1H2K   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2L   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
REMARK 900 RELATED ID: 1H2M   RELATED DB: PDB
REMARK 900  FACTOR INHIBITING HIF-1 ALPHA IN COMPLEX
REMARK 900  WITH HIF-1 ALPHA FRAGMENT PEPTIDE
DBREF  1H2N A    1   349  SWS    Q969Q7   Q969Q7           1    349
SEQRES   1 A  349  MET ALA ALA THR ALA ALA GLU ALA VAL ALA SER GLY SER
SEQRES   2 A  349  GLY GLU PRO ARG GLU GLU ALA GLY ALA LEU GLY PRO ALA
SEQRES   3 A  349  TRP ASP GLU SER GLN LEU ARG SER TYR SER PHE PRO THR
SEQRES   4 A  349  ARG PRO ILE PRO ARG LEU SER GLN SER ASP PRO ARG ALA
SEQRES   5 A  349  GLU GLU LEU ILE GLU ASN GLU GLU PRO VAL VAL LEU THR
SEQRES   6 A  349  ASP THR ASN LEU VAL TYR PRO ALA LEU LYS TRP ASP LEU
SEQRES   7 A  349  GLU TYR LEU GLN GLU ASN ILE GLY ASN GLY ASP PHE SER
SEQRES   8 A  349  VAL TYR SER ALA SER THR HIS LYS PHE LEU TYR TYR ASP
SEQRES   9 A  349  GLU LYS LYS MET ALA ASN PHE GLN ASN PHE LYS PRO ARG
SEQRES  10 A  349  SER ASN ARG GLU GLU MET LYS PHE HIS GLU PHE VAL GLU
SEQRES  11 A  349  LYS LEU GLN ASP ILE GLN GLN ARG GLY GLY GLU GLU ARG
SEQRES  12 A  349  LEU TYR LEU GLN GLN THR LEU ASN ASP THR VAL GLY ARG
SEQRES  13 A  349  LYS ILE VAL MET ASP PHE LEU GLY PHE ASN TRP ASN TRP
SEQRES  14 A  349  ILE ASN LYS GLN GLN GLY LYS ARG GLY TRP GLY GLN LEU
SEQRES  15 A  349  THR SER ASN LEU LEU LEU ILE GLY MET GLU GLY ASN VAL
SEQRES  16 A  349  THR PRO ALA HIS TYR ASP GLU GLN GLN ASN PHE PHE ALA
SEQRES  17 A  349  GLN ILE LYS GLY TYR LYS ARG CYS ILE LEU PHE PRO PRO
SEQRES  18 A  349  ASP GLN PHE GLU CYS LEU TYR PRO TYR PRO VAL HIS HIS
SEQRES  19 A  349  PRO CYS ASP ARG GLN SER GLN VAL ASP PHE ASP ASN PRO
SEQRES  20 A  349  ASP TYR GLU ARG PHE PRO ASN PHE GLN ASN VAL VAL GLY
SEQRES  21 A  349  TYR GLU THR VAL VAL GLY PRO GLY ASP VAL LEU TYR ILE
SEQRES  22 A  349  PRO MET TYR TRP TRP HIS HIS ILE GLU SER LEU LEU ASN
SEQRES  23 A  349  GLY GLY ILE THR ILE THR VAL ASN PHE TRP TYR LYS GLY
SEQRES  24 A  349  ALA PRO THR PRO LYS ARG ILE GLU TYR PRO LEU LYS ALA
SEQRES  25 A  349  HIS GLN LYS VAL ALA ILE MET ARG ASN ILE GLU LYS MET
SEQRES  26 A  349  LEU GLY GLU ALA LEU GLY ASN PRO GLN GLU VAL GLY PRO
SEQRES  27 A  349  LEU LEU ASN THR MET ILE LYS GLY ARG TYR ASN
HET    FE2  A1350       1
HET    AKG  A1351      10
HET    SO4  A1352       5
HET    SO4  A1353       5
HET    SO4  A1354       5
HETNAM     FE2 FE (II) ION
HETNAM     AKG 2-OXYGLUTARIC ACID
HETNAM     SO4 SULFATE ION
FORMUL   3  FE2    FE1 2+
FORMUL   4  AKG    C5 H6 O5
FORMUL   5  SO4    3(O4 S1 2-)
FORMUL   6  HOH   *3(H2 O1)
HELIX    1   1 ASP A   28  LEU A   32  5                                   5
HELIX    2   2 ASP A   49  ASN A   58  1                                  10
HELIX    3   3 VAL A   70  TRP A   76  5                                   7
HELIX    4   4 ASP A   77  ILE A   85  1                                   9
HELIX    5   5 ASP A  104  GLN A  112  5                                   9
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HELIX    6   6 PHE A  125  ARG A  138  1                                          14
HELIX    7   7 GLY A  155  GLY A  164  1                                          10
HELIX    8   8 ASN A  166  ARG A  177  1                                          12
HELIX    9   9 PRO A  220  ASP A  222  5                                           3
HELIX   10  10 GLN A  223  TYR A  228  1                                           6
HELIX   11  11 PHE A  252  VAL A  258  5                                           7
HELIX   12  12 LYS A  311  GLY A  331  1                                          21
HELIX   13  13 ASN A  332  GLN A  334  5                                           3
HELIX   14  14 GLU A  335  LYS A  345  1                                          11
SHEET    1  AA 5 THR A  39   PRO A  41   0
SHEET    2  AA 5 GLY A 260   VAL A 265   1  O  GLY A 260   N  ARG A  40
SHEET    3  AA 5 LYS A 214   PHE A 219  -1  O  LYS A 214   N  VAL A 265
SHEET    4  AA 5 TRP A 278   SER A 283  -1  O  TRP A 278   N  PHE A 219
SHEET    5  AA 5 VAL A 195   HIS A 199  -1  O  THR A 196   N  ILE A 281
SHEET    1  AB 6 ARG A  44   LEU A  45   0
SHEET    2  AB 6 VAL A  62   LEU A  64   1  O  VAL A  63   N  LEU A  45
SHEET    3  AB 6 VAL A 270   ILE A 273  -1  O  VAL A 270   N  LEU A  64
SHEET    4  AB 6 GLN A 203   LYS A 211  -1  O  ASN A 205   N  ILE A 273
SHEET    5  AB 6 THR A 290   LYS A 298  -1  O  ILE A 291   N  ILE A 210
SHEET    6  AB 6 LEU A 182   SER A 184  -1  N  THR A 183   O  TRP A 296
SHEET    1  AC 9 ARG A  44   LEU A  45   0
SHEET    2  AC 9 VAL A  62   LEU A  64   1  O  VAL A  63   N  LEU A  45
SHEET    3  AC 9 VAL A 270   ILE A 273  -1  O  VAL A 270   N  LEU A  64
SHEET    4  AC 9 GLN A 203   LYS A 211  -1  O  ASN A 205   N  ILE A 273
SHEET    5  AC 9 THR A 290   LYS A 298  -1  O  ILE A 291   N  ILE A 210
SHEET    6  AC 9 LEU A 186   GLY A 190  -1  O  LEU A 186   N  ASN A 294
SHEET    7  AC 9 ARG A 143   THR A 149  -1  O  LEU A 146   N  ILE A 189
SHEET    8  AC 9 ASP A  89   ALA A  95  -1  O  SER A  91   N  GLN A 147
SHEET    9  AC 9 SER A 118   LYS A 124  -1  O  ASN A 119   N  SER A  94
LINK         FE   FE2 A1350                 NE2 HIS A 199     1555   1555
LINK         FE   FE2 A1350                 OD2 ASP A 201     1555   1555
LINK         FE   FE2 A1350                 NE2 HIS A 279     1555   1555
LINK         FE   FE2 A1350                 O1  AKG A1351     1555   1555
LINK         FE   FE2 A1350                 O5  AKG A1351     1555   1555
CISPEP   1 TYR A  308     PRO A  309          0         2.48
SITE     1 FEA  3 HIS A 199  ASP A 201  HIS A 279
SITE     1 AKG 13 TYR A 145  LEU A 188  THR A 196  HIS A 199
SITE     2 AKG 13 ASP A 201  ASN A 205  PHE A 207  LYS A 214
SITE     3 AKG 13 HIS A 279  ILE A 281  ASN A 294  TRP A 296
SITE     4 AKG 13 HOH Z   1
SITE     1 SA1  4 ARG A 138  GLY A 140  GLU A 141  GLU A 142
SITE     1 SA2  5 ARG A 143  GLU A 192  GLY A 193  LEU A 285
SITE     2 SA2  5 ASN A 286
SITE     1 SA3  4 LYS A 107  GLU A 202  ARG A 320  LYS A 324
CRYST1   86.342   86.342  146.732  90.00  90.00  90.00 P 41 21 2     8
ORIGX1      1.000000  0.000000  0.000000        0.00000
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.011582  0.000000  0.000000        0.00000
SCALE2      0.000000  0.011582  0.000000        0.00000
SCALE3      0.000000  0.000000  0.006815        0.00000
ATOM     1  N   GLU A  15       8.558  32.684   9.824  1.00 41.85           N
ATOM     2  CA  GLU A  15       7.178  32.135   9.672  1.00 42.19           C
ATOM     3  C   GLU A  15       7.180  30.645   9.998  1.00 42.19           C
ATOM     4  O   GLU A  15       7.959  29.895   9.424  1.00 42.28           O
ATOM     5  CB  GLU A  15       6.661  32.366   8.258  1.00 42.28           C
ATOM     6  N   PRO A  16       6.281  30.198  10.866  1.00 42.29           N
ATOM     7  CA  PRO A  16       6.376  28.826  11.391  1.00 42.53           C
ATOM     8  C   PRO A  16       6.351  27.762  10.307  1.00 42.54           C
ATOM     9  O   PRO A  16       5.571  27.819   9.369  1.00 42.92           O
ATOM    10  CB  PRO A  16       5.172  28.713  12.337  1.00 42.63           C
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ATOM     11  CG  PRO A  16       4.749  30.155  12.612  1.00 42.41           C
ATOM     12  CD  PRO A  16       5.103  30.916  11.382  1.00 42.22           C
ATOM     13  N   ARG A  17       7.231  26.791  10.446  1.00 42.51           N
ATOM     14  CA  ARG A  17       7.337  25.723   9.478  1.00 42.62           C
ATOM     15  C   ARG A  17       6.095  24.856   9.527  1.00 42.85           C
ATOM     16  O   ARG A  17       5.492  24.705  10.587  1.00 43.51           O
ATOM     17  CB  ARG A  17       8.505  24.800   9.845  1.00 42.50           C
ATOM     18  CG  ARG A  17       9.871  25.434   9.859  1.00 42.22           C
ATOM     19  CD  ARG A  17      10.995  24.466  10.228  1.00 42.12           C
ATOM     20  NE  ARG A  17      11.085  24.138  11.656  1.00 42.49           N
ATOM     21  CZ  ARG A  17      11.588  24.943  12.607  1.00 42.43           C
ATOM     22  NH1 ARG A  17      12.033  26.158  12.316  1.00 42.11           N
ATOM     23  NH2 ARG A  17      11.649  24.529  13.869  1.00 42.25           N
ATOM     24  N   GLU A  18       5.742  24.242   8.404  1.00 42.60           N
ATOM     25  CA  GLU A  18       4.662  23.268   8.405  1.00 42.36           C
ATOM     26  C   GLU A  18       5.203  21.870   8.728  1.00 41.90           C
ATOM     27  O   GLU A  18       6.249  21.472   8.216  1.00 41.98           O
ATOM     28  CB  GLU A  18       3.988  23.224   7.041  1.00 42.57           C
ATOM     29  CG  GLU A  18       3.363  24.537   6.620  1.00 43.60           C
ATOM     30  CD  GLU A  18       1.993  24.756   7.233  1.00 45.11           C
ATOM     31  OE1 GLU A  18       1.365  23.766   7.686  1.00 45.48           O
ATOM     32  OE2 GLU A  18       1.546  25.926   7.253  1.00 46.49           O
ATOM     33  N   GLU A  19       4.487  21.133   9.578  1.00 41.27           N
ATOM     34  CA  GLU A  19       4.806  19.737   9.894  1.00 40.61           C
ATOM     35  C   GLU A  19       4.478  18.802   8.748  1.00 39.73           C
ATOM     36  O   GLU A  19       3.424  18.915   8.137  1.00 39.76           O
ATOM     37  CB  GLU A  19       4.024  19.299  11.128  1.00 40.72           C
ATOM     38  CG  GLU A  19       4.507  20.034  12.361  1.00 42.24           C
ATOM     39  CD  GLU A  19       4.358  19.278  13.668  1.00 44.37           C
ATOM     40  OE1 GLU A  19       3.852  18.127  13.680  1.00 46.17           O
ATOM     41  OE2 GLU A  19       4.769  19.863  14.700  1.00 45.44           O
ATOM     42  N   ALA A  20       5.369  17.859   8.478  1.00 38.99           N
ATOM     43  CA  ALA A  20       5.164  16.922   7.390  1.00 38.71           C
ATOM     44  C   ALA A  20       3.831  16.232   7.542  1.00 38.51           C
ATOM     45  O   ALA A  20       3.391  15.933   8.649  1.00 38.80           O
ATOM     46  CB  ALA A  20       6.280  15.895   7.328  1.00 38.51           C
ATOM     47  N   GLY A  21       3.180  15.991   6.419  1.00 38.03           N
ATOM     48  CA  GLY A  21       1.924  15.290   6.449  1.00 38.11           C
ATOM     49  C   GLY A  21       0.746  16.205   6.682  1.00 38.19           C
ATOM     50  O   GLY A  21      -0.328  15.743   7.049  1.00 38.25           O
ATOM     51  N   ALA A  22       0.941  17.497   6.447  1.00 38.40           N
ATOM     52  CA  ALA A  22      -0.130  18.472   6.571  1.00 38.50           C
ATOM     53  C   ALA A  22      -0.725  18.413   7.960  1.00 38.60           C
ATOM     54  O   ALA A  22      -1.930  18.547   8.142  1.00 38.65           O
ATOM     55  CB  ALA A  22      -1.196  18.242   5.520  1.00 38.61           C
ATOM     56  N   LEU A  23       0.135  18.206   8.946  1.00 38.75           N
ATOM     57  CA  LEU A  23      -0.297  18.257  10.330  1.00 38.82           C
ATOM     58  C   LEU A  23      -0.321  19.684  10.843  1.00 38.78           C
ATOM     59  O   LEU A  23      -0.525  19.919  12.030  1.00 38.74           O
ATOM     60  CB  LEU A  23       0.597  17.392  11.193  1.00 38.77           C
ATOM     61  CG  LEU A  23       0.421  15.952  10.736  1.00 39.03           C
ATOM     62  CD1 LEU A  23       1.203  14.958  11.579  1.00 39.08           C
ATOM     63  CD2 LEU A  23      -1.070  15.636  10.750  1.00 39.43           C
ATOM     64  N   GLY A  24      -0.094  20.636   9.947  1.00 38.75           N
ATOM     65  CA  GLY A  24      -0.248  22.025  10.298  1.00 38.79           C
ATOM     66  C   GLY A  24       0.972  22.669  10.861  1.00 38.90           C
ATOM     67  O   GLY A  24       2.042  22.084  10.961  1.00 39.06           O
ATOM     68  N   PRO A  25       0.791  23.906  11.267  1.00 39.19           N
ATOM     69  CA  PRO A  25       1.903  24.682  11.778  1.00 39.35           C
ATOM     70  C   PRO A  25       2.332  24.037  13.074  1.00 39.62           C
ATOM     71  O   PRO A  25       1.492  23.633  13.871  1.00 39.48           O
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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 72 | CB | PRO | A | 25 | 1.299 | 26.062 | 12.019 | 1.00 | 39.24 | C |
| ATOM | 73 | CG | PRO | A | 25 | -0.142 | 25.920 | 11.961 | 1.00 | 38.71 | C |
| ATOM | 74 | CD | PRO | A | 25 | -0.490 | 24.616 | 11.365 | 1.00 | 39.17 | C |
| ATOM | 75 | N | ALA | A | 26 | 3.631 | 23.899 | 13.252 | 1.00 | 40.22 | N |
| ATOM | 76 | CA | ALA | A | 26 | 4.170 | 23.342 | 14.476 | 1.00 | 40.79 | C |
| ATOM | 77 | C | ALA | A | 26 | 3.930 | 24.294 | 15.666 | 1.00 | 41.07 | C |
| ATOM | 78 | O | ALA | A | 26 | 3.769 | 23.837 | 16.797 | 1.00 | 41.57 | O |
| ATOM | 79 | CB | ALA | A | 26 | 5.633 | 23.068 | 14.300 | 1.00 | 40.98 | C |
| ATOM | 80 | N | TRP | A | 27 | 3.931 | 25.605 | 15.429 | 1.00 | 40.80 | N |
| ATOM | 81 | CA | TRP | A | 27 | 3.543 | 26.552 | 16.477 | 1.00 | 40.67 | C |
| ATOM | 82 | C | TRP | A | 27 | 2.982 | 27.848 | 15.880 | 1.00 | 40.33 | C |
| ATOM | 83 | O | TRP | A | 27 | 2.777 | 27.940 | 14.675 | 1.00 | 40.13 | O |
| ATOM | 84 | CB | TRP | A | 27 | 4.742 | 26.860 | 17.358 | 1.00 | 40.70 | C |
| ATOM | 85 | CG | TRP | A | 27 | 5.942 | 27.014 | 16.558 | 1.00 | 41.36 | C |
| ATOM | 86 | CD1 | TRP | A | 27 | 6.762 | 26.023 | 16.074 | 1.00 | 43.03 | C |
| ATOM | 87 | CD2 | TRP | A | 27 | 6.466 | 28.233 | 16.084 | 1.00 | 40.41 | C |
| ATOM | 88 | NE1 | TRP | A | 27 | 7.788 | 26.579 | 15.344 | 1.00 | 42.65 | N |
| ATOM | 89 | CE2 | TRP | A | 27 | 7.618 | 27.938 | 15.331 | 1.00 | 41.20 | C |
| ATOM | 90 | CE3 | TRP | A | 27 | 6.081 | 29.555 | 16.223 | 1.00 | 40.47 | C |
| ATOM | 91 | CZ2 | TRP | A | 27 | 8.370 | 28.912 | 14.732 | 1.00 | 41.10 | C |
| ATOM | 92 | CZ3 | TRP | A | 27 | 6.827 | 30.514 | 15.640 | 1.00 | 41.11 | C |
| ATOM | 93 | CH2 | TRP | A | 27 | 7.962 | 30.198 | 14.900 | 1.00 | 41.57 | C |
| ATOM | 94 | N | ASP | A | 28 | 2.677 | 28.830 | 16.723 | 1.00 | 39.99 | N |
| ATOM | 95 | CA | ASP | A | 28 | 2.322 | 30.143 | 16.209 | 1.00 | 39.78 | C |
| ATOM | 96 | C | ASP | A | 28 | 2.802 | 31.257 | 17.121 | 1.00 | 39.17 | C |
| ATOM | 97 | O | ASP | A | 28 | 3.227 | 31.013 | 18.240 | 1.00 | 39.00 | O |
| ATOM | 98 | CB | ASP | A | 28 | 0.826 | 30.254 | 15.981 | 1.00 | 40.16 | C |
| ATOM | 99 | CG | ASP | A | 28 | 0.066 | 30.380 | 17.258 | 1.00 | 40.79 | C |
| ATOM | 100 | OD1 | ASP | A | 28 | 0.044 | 31.496 | 17.821 | 1.00 | 41.30 | O |
| ATOM | 101 | OD2 | ASP | A | 28 | -0.531 | 29.414 | 17.774 | 1.00 | 42.25 | O |
| ATOM | 102 | N | GLU | A | 29 | 2.720 | 32.486 | 16.624 | 1.00 | 38.73 | N |
| ATOM | 103 | CA | GLU | A | 29 | 3.223 | 33.663 | 17.341 | 1.00 | 38.23 | C |
| ATOM | 104 | C | GLU | A | 29 | 2.739 | 33.764 | 18.781 | 1.00 | 37.69 | C |
| ATOM | 105 | O | GLU | A | 29 | 3.492 | 34.131 | 19.664 | 1.00 | 37.34 | O |
| ATOM | 106 | CB | GLU | A | 29 | 2.834 | 34.924 | 16.594 | 1.00 | 38.20 | C |
| ATOM | 107 | N | SER | A | 30 | 1.482 | 33.418 | 19.012 | 1.00 | 37.46 | N |
| ATOM | 108 | CA | SER | A | 30 | 0.874 | 33.583 | 20.324 | 1.00 | 37.18 | C |
| ATOM | 109 | C | SER | A | 30 | 1.562 | 32.774 | 21.399 | 1.00 | 36.93 | C |
| ATOM | 110 | O | SER | A | 30 | 1.282 | 32.949 | 22.577 | 1.00 | 36.82 | O |
| ATOM | 111 | CB | SER | A | 30 | -0.595 | 33.164 | 20.284 | 1.00 | 37.23 | C |
| ATOM | 112 | OG | SER | A | 30 | -0.744 | 31.792 | 20.619 | 1.00 | 36.97 | O |
| ATOM | 113 | N | GLN | A | 31 | 2.441 | 31.867 | 20.999 | 1.00 | 36.85 | N |
| ATOM | 114 | CA | GLN | A | 31 | 3.128 | 31.021 | 21.961 | 1.00 | 36.77 | C |
| ATOM | 115 | C | GLN | A | 31 | 4.445 | 31.636 | 22.340 | 1.00 | 36.59 | C |
| ATOM | 116 | O | GLN | A | 31 | 5.141 | 31.127 | 23.220 | 1.00 | 36.74 | O |
| ATOM | 117 | CB | GLN | A | 31 | 3.366 | 29.621 | 21.395 | 1.00 | 36.71 | C |
| ATOM | 118 | CG | GLN | A | 31 | 2.084 | 28.828 | 21.234 | 1.00 | 36.97 | C |
| ATOM | 119 | CD | GLN | A | 31 | 2.282 | 27.497 | 20.560 | 1.00 | 36.68 | C |
| ATOM | 120 | OE1 | GLN | A | 31 | 2.133 | 27.386 | 19.346 | 1.00 | 36.62 | O |
| ATOM | 121 | NE2 | GLN | A | 31 | 2.601 | 26.478 | 21.343 | 1.00 | 36.85 | N |
| ATOM | 122 | N | LEU | A | 32 | 4.794 | 32.726 | 21.670 | 1.00 | 36.32 | N |
| ATOM | 123 | CA | LEU | A | 32 | 6.050 | 33.381 | 21.942 | 1.00 | 36.17 | C |
| ATOM | 124 | C | LEU | A | 32 | 5.817 | 34.498 | 22.921 | 1.00 | 36.09 | C |
| ATOM | 125 | O | LEU | A | 32 | 4.837 | 35.233 | 22.815 | 1.00 | 36.18 | O |
| ATOM | 126 | CB | LEU | A | 32 | 6.673 | 33.928 | 20.664 | 1.00 | 36.07 | C |
| ATOM | 127 | CG | LEU | A | 32 | 6.990 | 32.871 | 19.604 | 1.00 | 36.72 | C |
| ATOM | 128 | CD1 | LEU | A | 32 | 7.747 | 33.457 | 18.453 | 1.00 | 36.96 | C |
| ATOM | 129 | CD2 | LEU | A | 32 | 7.797 | 31.744 | 20.161 | 1.00 | 37.31 | C |
| ATOM | 130 | N | ARG | A | 33 | 6.700 | 34.576 | 23.908 | 1.00 | 35.99 | N |
| ATOM | 131 | CA | ARG | A | 33 | 6.713 | 35.671 | 24.851 | 1.00 | 36.15 | C |
| ATOM | 132 | C | ARG | A | 33 | 7.171 | 36.941 | 24.130 | 1.00 | 35.95 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 133 | O | ARG | A | 33 | 7.950 | 36.888 | 23.188 | 1.00 35.75 | O |
| ATOM | 134 | CB | ARG | A | 33 | 7.671 | 35.350 | 25.991 | 1.00 36.41 | C |
| ATOM | 135 | CG | ARG | A | 33 | 7.210 | 34.204 | 26.854 | 1.00 36.76 | C |
| ATOM | 136 | CD | ARG | A | 33 | 8.082 | 33.948 | 28.070 | 1.00 36.81 | C |
| ATOM | 137 | NE | ARG | A | 33 | 7.479 | 32.927 | 28.923 | 1.00 37.39 | N |
| ATOM | 138 | CZ | ARG | A | 33 | 6.501 | 33.160 | 29.785 | 1.00 37.61 | C |
| ATOM | 139 | NH1 | ARG | A | 33 | 6.027 | 34.385 | 29.931 | 1.00 37.75 | N |
| ATOM | 140 | NH2 | ARG | A | 33 | 6.001 | 32.171 | 30.513 | 1.00 38.47 | N |
| ATOM | 141 | N | SER | A | 34 | 6.707 | 38.088 | 24.588 | 1.00 35.92 | N |
| ATOM | 142 | CA | SER | A | 34 | 7.017 | 39.331 | 23.902 | 1.00 36.05 | C |
| ATOM | 143 | C | SER | A | 34 | 8.044 | 40.146 | 24.671 | 1.00 35.47 | C |
| ATOM | 144 | O | SER | A | 34 | 7.940 | 40.311 | 25.884 | 1.00 35.41 | O |
| ATOM | 145 | CB | SER | A | 34 | 5.732 | 40.120 | 23.691 | 1.00 36.27 | C |
| ATOM | 146 | OG | SER | A | 34 | 5.046 | 40.253 | 24.920 | 1.00 37.99 | O |
| ATOM | 147 | N | TYR | A | 35 | 9.031 | 40.655 | 23.945 | 1.00 35.01 | N |
| ATOM | 148 | CA | TYR | A | 35 | 10.140 | 41.370 | 24.543 | 1.00 34.69 | C |
| ATOM | 149 | C | TYR | A | 35 | 10.400 | 42.693 | 23.853 | 1.00 34.59 | C |
| ATOM | 150 | O | TYR | A | 35 | 9.841 | 42.989 | 22.813 | 1.00 34.45 | O |
| ATOM | 151 | CB | TYR | A | 35 | 11.384 | 40.501 | 24.469 | 1.00 34.71 | C |
| ATOM | 152 | CG | TYR | A | 35 | 11.228 | 39.222 | 25.232 | 1.00 34.43 | C |
| ATOM | 153 | CD1 | TYR | A | 35 | 10.928 | 39.246 | 26.573 | 1.00 33.87 | C |
| ATOM | 154 | CD2 | TYR | A | 35 | 11.350 | 37.986 | 24.602 | 1.00 35.32 | C |
| ATOM | 155 | CE1 | TYR | A | 35 | 10.775 | 38.087 | 27.285 | 1.00 34.96 | C |
| ATOM | 156 | CE2 | TYR | A | 35 | 11.192 | 36.807 | 25.309 | 1.00 35.50 | C |
| ATOM | 157 | CZ | TYR | A | 35 | 10.904 | 36.865 | 26.653 | 1.00 35.16 | C |
| ATOM | 158 | OH | TYR | A | 35 | 10.742 | 35.709 | 27.376 | 1.00 34.77 | O |
| ATOM | 159 | N | SER | A | 36 | 11.290 | 43.481 | 24.429 | 1.00 34.77 | N |
| ATOM | 160 | CA | SER | A | 36 | 11.572 | 44.814 | 23.924 | 1.00 34.74 | C |
| ATOM | 161 | C | SER | A | 36 | 12.567 | 44.926 | 22.771 | 1.00 34.30 | C |
| ATOM | 162 | O | SER | A | 36 | 12.805 | 46.011 | 22.287 | 1.00 34.23 | O |
| ATOM | 163 | CB | SER | A | 36 | 12.127 | 45.627 | 25.077 | 1.00 34.91 | C |
| ATOM | 164 | OG | SER | A | 36 | 13.395 | 45.116 | 25.449 | 1.00 35.56 | O |
| ATOM | 165 | N | PHE | A | 37 | 13.155 | 43.838 | 22.318 | 1.00 34.15 | N |
| ATOM | 166 | CA | PHE | A | 37 | 14.193 | 43.963 | 21.306 | 1.00 34.11 | C |
| ATOM | 167 | C | PHE | A | 37 | 13.969 | 43.177 | 20.044 | 1.00 34.07 | C |
| ATOM | 168 | O | PHE | A | 37 | 13.356 | 42.109 | 20.017 | 1.00 33.98 | O |
| ATOM | 169 | CB | PHE | A | 37 | 15.514 | 43.479 | 21.867 | 1.00 34.08 | C |
| ATOM | 170 | CG | PHE | A | 37 | 15.417 | 42.147 | 22.438 | 1.00 34.33 | C |
| ATOM | 171 | CD1 | PHE | A | 37 | 15.445 | 41.034 | 21.621 | 1.00 35.66 | C |
| ATOM | 172 | CD2 | PHE | A | 37 | 15.208 | 41.990 | 23.777 | 1.00 35.42 | C |
| ATOM | 173 | CE1 | PHE | A | 37 | 15.320 | 39.782 | 22.143 | 1.00 35.73 | C |
| ATOM | 174 | CE2 | PHE | A | 37 | 15.084 | 40.736 | 24.317 | 1.00 36.14 | C |
| ATOM | 175 | CZ | PHE | A | 37 | 15.141 | 39.628 | 23.497 | 1.00 36.55 | C |
| ATOM | 176 | N | PRO | A | 38 | 14.565 | 43.682 | 18.991 | 1.00 33.95 | N |
| ATOM | 177 | CA | PRO | A | 38 | 14.474 | 43.028 | 17.704 | 1.00 33.91 | C |
| ATOM | 178 | C | PRO | A | 38 | 15.445 | 41.878 | 17.640 | 1.00 33.74 | C |
| ATOM | 179 | O | PRO | A | 38 | 16.366 | 41.803 | 18.441 | 1.00 33.82 | O |
| ATOM | 180 | CB | PRO | A | 38 | 14.887 | 44.133 | 16.751 | 1.00 34.03 | C |
| ATOM | 181 | CG | PRO | A | 38 | 15.874 | 44.935 | 17.548 | 1.00 33.99 | C |
| ATOM | 182 | CD | PRO | A | 38 | 15.385 | 44.903 | 18.945 | 1.00 33.80 | C |
| ATOM | 183 | N | THR | A | 39 | 15.233 | 40.996 | 16.678 | 1.00 34.02 | N |
| ATOM | 184 | CA | THR | A | 39 | 16.089 | 39.844 | 16.464 | 1.00 34.00 | C |
| ATOM | 185 | C | THR | A | 39 | 16.035 | 39.490 | 15.008 | 1.00 34.09 | C |
| ATOM | 186 | O | THR | A | 39 | 15.137 | 39.894 | 14.311 | 1.00 34.05 | O |
| ATOM | 187 | CB | THR | A | 39 | 15.563 | 38.637 | 17.201 | 1.00 33.94 | C |
| ATOM | 188 | OG1 | THR | A | 39 | 14.250 | 38.336 | 16.714 | 1.00 34.18 | O |
| ATOM | 189 | CG2 | THR | A | 39 | 15.338 | 38.915 | 18.642 | 1.00 34.09 | C |
| ATOM | 190 | N | ARG | A | 40 | 16.992 | 38.695 | 14.576 | 1.00 34.62 | N |
| ATOM | 191 | CA | ARG | A | 40 | 17.066 | 38.204 | 13.228 | 1.00 35.13 | C |
| ATOM | 192 | C | ARG | A | 40 | 17.100 | 36.721 | 13.361 | 1.00 35.17 | C |
| ATOM | 193 | O | ARG | A | 40 | 17.419 | 36.189 | 14.434 | 1.00 34.96 | O |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 194 | CB | ARG | A | 40 | 18.352 | 38.649 | 12.568 | 1.00 | 35.54 | C |
| ATOM | 195 | CG | ARG | A | 40 | 18.358 | 40.103 | 12.287 | 1.00 | 38.87 | C |
| ATOM | 196 | CD | ARG | A | 40 | 16.975 | 40.597 | 11.893 | 1.00 | 42.88 | C |
| ATOM | 197 | NE | ARG | A | 40 | 16.737 | 40.908 | 10.489 | 1.00 | 44.50 | N |
| ATOM | 198 | CZ | ARG | A | 40 | 15.554 | 41.298 | 10.076 | 1.00 | 46.73 | C |
| ATOM | 199 | NH1 | ARG | A | 40 | 14.574 | 41.350 | 10.974 | 1.00 | 46.73 | N |
| ATOM | 200 | NH2 | ARG | A | 40 | 15.334 | 41.636 | 8.802 | 1.00 | 48.87 | N |
| ATOM | 201 | N | PRO | A | 41 | 16.775 | 36.026 | 12.285 | 1.00 | 35.20 | N |
| ATOM | 202 | CA | PRO | A | 41 | 16.749 | 34.579 | 12.348 | 1.00 | 35.24 | C |
| ATOM | 203 | C | PRO | A | 41 | 18.114 | 33.973 | 12.275 | 1.00 | 35.10 | C |
| ATOM | 204 | O | PRO | A | 41 | 18.995 | 34.455 | 11.573 | 1.00 | 35.96 | O |
| ATOM | 205 | CB | PRO | A | 41 | 16.003 | 34.208 | 11.079 | 1.00 | 35.27 | C |
| ATOM | 206 | CG | PRO | A | 41 | 15.408 | 35.453 | 10.640 | 1.00 | 34.93 | C |
| ATOM | 207 | CD | PRO | A | 41 | 16.381 | 36.494 | 10.953 | 1.00 | 34.81 | C |
| ATOM | 208 | N | ILE | A | 42 | 18.277 | 32.910 | 13.022 | 1.00 | 34.55 | N |
| ATOM | 209 | CA | ILE | A | 42 | 19.435 | 32.099 | 12.909 | 1.00 | 34.29 | C |
| ATOM | 210 | C | ILE | A | 42 | 19.145 | 31.194 | 11.713 | 1.00 | 34.29 | C |
| ATOM | 211 | O | ILE | A | 42 | 18.035 | 30.654 | 11.598 | 1.00 | 34.38 | O |
| ATOM | 212 | CB | ILE | A | 42 | 19.545 | 31.258 | 14.150 | 1.00 | 34.14 | C |
| ATOM | 213 | CG1 | ILE | A | 42 | 19.742 | 32.152 | 15.368 | 1.00 | 34.83 | C |
| ATOM | 214 | CG2 | ILE | A | 42 | 20.679 | 30.297 | 14.016 | 1.00 | 34.41 | C |
| ATOM | 215 | CD1 | ILE | A | 42 | 19.479 | 31.467 | 16.678 | 1.00 | 35.37 | C |
| ATOM | 216 | N | PRO | A | 43 | 20.127 | 31.010 | 10.836 | 1.00 | 33.80 | N |
| ATOM | 217 | CA | PRO | A | 43 | 19.982 | 30.122 | 9.686 | 1.00 | 33.62 | C |
| ATOM | 218 | C | PRO | A | 43 | 19.714 | 28.676 | 10.066 | 1.00 | 33.65 | C |
| ATOM | 219 | O | PRO | A | 43 | 20.320 | 28.198 | 11.015 | 1.00 | 33.60 | O |
| ATOM | 220 | CB | PRO | A | 43 | 21.366 | 30.174 | 9.043 | 1.00 | 33.63 | C |
| ATOM | 221 | CG | PRO | A | 43 | 21.986 | 31.385 | 9.543 | 1.00 | 33.11 | C |
| ATOM | 222 | CD | PRO | A | 43 | 21.455 | 31.630 | 10.882 | 1.00 | 33.51 | C |
| ATOM | 223 | N | ARG | A | 44 | 18.820 | 28.007 | 9.341 | 1.00 | 33.86 | N |
| ATOM | 224 | CA | ARG | A | 44 | 18.597 | 26.572 | 9.486 | 1.00 | 34.00 | C |
| ATOM | 225 | C | ARG | A | 44 | 19.176 | 25.968 | 8.247 | 1.00 | 33.87 | C |
| ATOM | 226 | O | ARG | A | 44 | 18.783 | 26.319 | 7.152 | 1.00 | 33.76 | O |
| ATOM | 227 | CB | ARG | A | 44 | 17.125 | 26.185 | 9.520 | 1.00 | 34.10 | C |
| ATOM | 228 | CG | ARG | A | 44 | 16.301 | 26.879 | 10.577 | 1.00 | 35.44 | C |
| ATOM | 229 | CD | ARG | A | 44 | 14.781 | 26.505 | 10.583 | 1.00 | 37.36 | C |
| ATOM | 230 | NE | ARG | A | 44 | 14.415 | 25.108 | 10.265 | 1.00 | 37.59 | N |
| ATOM | 231 | CZ | ARG | A | 44 | 14.237 | 24.144 | 11.187 | 1.00 | 39.71 | C |
| ATOM | 232 | NH1 | ARG | A | 44 | 14.429 | 24.396 | 12.487 | 1.00 | 39.94 | N |
| ATOM | 233 | NH2 | ARG | A | 44 | 13.876 | 22.915 | 10.821 | 1.00 | 40.07 | N |
| ATOM | 234 | N | LEU | A | 45 | 20.086 | 25.030 | 8.407 | 1.00 | 33.98 | N |
| ATOM | 235 | CA | LEU | A | 45 | 20.747 | 24.467 | 7.269 | 1.00 | 34.15 | C |
| ATOM | 236 | C | LEU | A | 45 | 20.950 | 22.995 | 7.389 | 1.00 | 34.37 | C |
| ATOM | 237 | O | LEU | A | 45 | 20.901 | 22.453 | 8.486 | 1.00 | 34.52 | O |
| ATOM | 238 | CB | LEU | A | 45 | 22.116 | 25.090 | 7.183 | 1.00 | 34.25 | C |
| ATOM | 239 | CG | LEU | A | 45 | 22.080 | 26.576 | 6.905 | 1.00 | 34.80 | C |
| ATOM | 240 | CD1 | LEU | A | 45 | 23.454 | 27.095 | 7.177 | 1.00 | 36.05 | C |
| ATOM | 241 | CD2 | LEU | A | 45 | 21.655 | 26.837 | 5.481 | 1.00 | 34.78 | C |
| ATOM | 242 | N | SER | A | 46 | 21.199 | 22.343 | 6.255 | 1.00 | 34.55 | N |
| ATOM | 243 | CA | SER | A | 46 | 21.549 | 20.949 | 6.306 | 1.00 | 34.60 | C |
| ATOM | 244 | C | SER | A | 46 | 22.985 | 20.838 | 6.681 | 1.00 | 34.89 | C |
| ATOM | 245 | O | SER | A | 46 | 23.826 | 21.671 | 6.383 | 1.00 | 34.54 | O |
| ATOM | 246 | CB | SER | A | 46 | 21.356 | 20.206 | 5.006 | 1.00 | 34.64 | C |
| ATOM | 247 | OG | SER | A | 46 | 22.231 | 19.090 | 4.989 | 1.00 | 33.61 | O |
| ATOM | 248 | N | GLN | A | 47 | 23.247 | 19.736 | 7.324 | 1.00 | 35.61 | N |
| ATOM | 249 | CA | GLN | A | 47 | 24.539 | 19.462 | 7.866 | 1.00 | 36.10 | C |
| ATOM | 250 | C | GLN | A | 47 | 25.565 | 19.368 | 6.746 | 1.00 | 35.96 | C |
| ATOM | 251 | O | GLN | A | 47 | 26.754 | 19.537 | 6.969 | 1.00 | 36.13 | O |
| ATOM | 252 | CB | GLN | A | 47 | 24.399 | 18.168 | 8.669 | 1.00 | 36.22 | C |
| ATOM | 253 | CG | GLN | A | 47 | 25.604 | 17.340 | 8.730 | 1.00 | 37.25 | C |
| ATOM | 254 | CD | GLN | A | 47 | 25.724 | 16.459 | 7.532 | 1.00 | 39.03 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 255 | OE1 | GLN | A | 47 | 24.766 | 16.306 | 6.759 | 1.00 | 38.79 | O |
| ATOM | 256 | NE2 | GLN | A | 47 | 26.902 | 15.872 | 7.354 | 1.00 | 41.44 | N |
| ATOM | 257 | N | SER | A | 48 | 25.088 | 19.146 | 5.531 | 1.00 | 35.87 | N |
| ATOM | 258 | CA | SER | A | 48 | 25.958 | 18.938 | 4.391 | 1.00 | 35.90 | C |
| ATOM | 259 | C | SER | A | 48 | 26.301 | 20.244 | 3.715 | 1.00 | 36.06 | C |
| ATOM | 260 | O | SER | A | 48 | 27.215 | 20.334 | 2.897 | 1.00 | 35.95 | O |
| ATOM | 261 | CB | SER | A | 48 | 25.214 | 18.073 | 3.402 | 1.00 | 35.97 | C |
| ATOM | 262 | OG | SER | A | 48 | 23.933 | 18.635 | 3.158 | 1.00 | 36.62 | O |
| ATOM | 263 | N | ASP | A | 49 | 25.552 | 21.266 | 4.075 | 1.00 | 36.34 | N |
| ATOM | 264 | CA | ASP | A | 49 | 25.701 | 22.564 | 3.491 | 1.00 | 36.65 | C |
| ATOM | 265 | C | ASP | A | 49 | 26.963 | 23.236 | 3.952 | 1.00 | 37.06 | C |
| ATOM | 266 | O | ASP | A | 49 | 27.114 | 23.507 | 5.138 | 1.00 | 37.24 | O |
| ATOM | 267 | CB | ASP | A | 49 | 24.545 | 23.405 | 3.953 | 1.00 | 36.80 | C |
| ATOM | 268 | CG | ASP | A | 49 | 24.441 | 24.674 | 3.206 | 1.00 | 37.08 | C |
| ATOM | 269 | OD1 | ASP | A | 49 | 25.490 | 25.217 | 2.810 | 1.00 | 37.38 | O |
| ATOM | 270 | OD2 | ASP | A | 49 | 23.343 | 25.187 | 2.953 | 1.00 | 38.64 | O |
| ATOM | 271 | N | PRO | A | 50 | 27.857 | 23.565 | 3.029 | 1.00 | 37.42 | N |
| ATOM | 272 | CA | PRO | A | 50 | 29.113 | 24.196 | 3.430 | 1.00 | 37.32 | C |
| ATOM | 273 | C | PRO | A | 50 | 28.881 | 25.413 | 4.298 | 1.00 | 37.46 | C |
| ATOM | 274 | O | PRO | A | 50 | 29.742 | 25.727 | 5.113 | 1.00 | 37.85 | O |
| ATOM | 275 | CB | PRO | A | 50 | 29.750 | 24.604 | 2.108 | 1.00 | 37.21 | C |
| ATOM | 276 | CG | PRO | A | 50 | 29.134 | 23.726 | 1.086 | 1.00 | 37.39 | C |
| ATOM | 277 | CD | PRO | A | 50 | 27.755 | 23.395 | 1.568 | 1.00 | 37.34 | C |
| ATOM | 278 | N | ARG | A | 51 | 27.743 | 26.081 | 4.162 | 1.00 | 37.64 | N |
| ATOM | 279 | CA | ARG | A | 51 | 27.535 | 27.301 | 4.932 | 1.00 | 38.06 | C |
| ATOM | 280 | C | ARG | A | 51 | 27.470 | 27.000 | 6.421 | 1.00 | 38.26 | C |
| ATOM | 281 | O | ARG | A | 51 | 27.920 | 27.798 | 7.250 | 1.00 | 38.47 | O |
| ATOM | 282 | CB | ARG | A | 51 | 26.282 | 28.055 | 4.470 | 1.00 | 38.14 | C |
| ATOM | 283 | CG | ARG | A | 51 | 26.418 | 28.692 | 3.059 | 1.00 | 38.89 | C |
| ATOM | 284 | CD | ARG | A | 51 | 25.117 | 29.259 | 2.455 | 1.00 | 39.65 | C |
| ATOM | 285 | NE | ARG | A | 51 | 24.121 | 28.211 | 2.175 | 1.00 | 41.25 | N |
| ATOM | 286 | CZ | ARG | A | 51 | 22.798 | 28.404 | 2.078 | 1.00 | 41.86 | C |
| ATOM | 287 | NH1 | ARG | A | 51 | 22.264 | 29.605 | 2.225 | 1.00 | 43.70 | N |
| ATOM | 288 | NH2 | ARG | A | 51 | 21.994 | 27.393 | 1.818 | 1.00 | 41.90 | N |
| ATOM | 289 | N | ALA | A | 52 | 26.936 | 25.837 | 6.770 | 1.00 | 38.26 | N |
| ATOM | 290 | CA | ALA | A | 52 | 26.807 | 25.499 | 8.171 | 1.00 | 38.30 | C |
| ATOM | 291 | C | ALA | A | 52 | 28.206 | 25.374 | 8.683 | 1.00 | 38.45 | C |
| ATOM | 292 | O | ALA | A | 52 | 28.572 | 25.922 | 9.732 | 1.00 | 38.37 | O |
| ATOM | 293 | CB | ALA | A | 52 | 26.085 | 24.208 | 8.344 | 1.00 | 38.25 | C |
| ATOM | 294 | N | GLU | A | 53 | 29.003 | 24.665 | 7.901 | 1.00 | 38.56 | N |
| ATOM | 295 | CA | GLU | A | 53 | 30.361 | 24.420 | 8.291 | 1.00 | 38.94 | C |
| ATOM | 296 | C | GLU | A | 53 | 31.145 | 25.717 | 8.484 | 1.00 | 39.00 | C |
| ATOM | 297 | O | GLU | A | 53 | 31.970 | 25.793 | 9.386 | 1.00 | 38.49 | O |
| ATOM | 298 | CB | GLU | A | 53 | 31.060 | 23.507 | 7.314 | 1.00 | 38.91 | C |
| ATOM | 299 | CG | GLU | A | 53 | 32.139 | 22.738 | 8.035 | 1.00 | 40.55 | C |
| ATOM | 300 | CD | GLU | A | 53 | 31.662 | 21.403 | 8.579 | 1.00 | 42.38 | C |
| ATOM | 301 | OE1 | GLU | A | 53 | 30.475 | 21.274 | 8.957 | 1.00 | 43.42 | O |
| ATOM | 302 | OE2 | GLU | A | 53 | 32.498 | 20.478 | 8.639 | 1.00 | 44.15 | O |
| ATOM | 303 | N | GLU | A | 54 | 30.897 | 26.737 | 7.662 | 1.00 | 39.21 | N |
| ATOM | 304 | CA | GLU | A | 54 | 31.592 | 28.004 | 7.870 | 1.00 | 39.44 | C |
| ATOM | 305 | C | GLU | A | 54 | 31.092 | 28.625 | 9.144 | 1.00 | 39.05 | C |
| ATOM | 306 | O | GLU | A | 54 | 31.848 | 29.262 | 9.869 | 1.00 | 39.51 | O |
| ATOM | 307 | CB | GLU | A | 54 | 31.337 | 29.023 | 6.772 | 1.00 | 39.59 | C |
| ATOM | 308 | CG | GLU | A | 54 | 31.940 | 28.693 | 5.433 | 1.00 | 41.75 | C |
| ATOM | 309 | CD | GLU | A | 54 | 31.098 | 29.263 | 4.302 | 1.00 | 44.74 | C |
| ATOM | 310 | OE1 | GLU | A | 54 | 30.546 | 30.379 | 4.509 | 1.00 | 46.67 | O |
| ATOM | 311 | OE2 | GLU | A | 54 | 30.972 | 28.596 | 3.234 | 1.00 | 44.49 | O |
| ATOM | 312 | N | LEU | A | 55 | 29.812 | 28.468 | 9.424 | 1.00 | 38.37 | N |
| ATOM | 313 | CA | LEU | A | 55 | 29.291 | 29.137 | 10.583 | 1.00 | 38.08 | C |
| ATOM | 314 | C | LEU | A | 55 | 29.906 | 28.613 | 11.847 | 1.00 | 37.88 | C |
| ATOM | 315 | O | LEU | A | 55 | 30.359 | 29.397 | 12.693 | 1.00 | 37.59 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 316 | CB | LEU | A | 55 | 27.789 | 29.006 | 10.648 | 1.00 | 38.28 | C |
| ATOM | 317 | CG | LEU | A | 55 | 27.142 | 29.846 | 9.564 | 1.00 | 37.79 | C |
| ATOM | 318 | CD1 | LEU | A | 55 | 25.722 | 29.443 | 9.409 | 1.00 | 38.31 | C |
| ATOM | 319 | CD2 | LEU | A | 55 | 27.233 | 31.279 | 9.951 | 1.00 | 37.31 | C |
| ATOM | 320 | N | ILE | A | 56 | 29.938 | 27.286 | 11.971 | 1.00 | 37.71 | N |
| ATOM | 321 | CA | ILE | A | 56 | 30.455 | 26.667 | 13.183 | 1.00 | 37.35 | C |
| ATOM | 322 | C | ILE | A | 56 | 31.912 | 26.988 | 13.321 | 1.00 | 37.30 | C |
| ATOM | 323 | O | ILE | A | 56 | 32.373 | 27.320 | 14.406 | 1.00 | 36.89 | O |
| ATOM | 324 | CB | ILE | A | 56 | 30.288 | 25.171 | 13.175 | 1.00 | 37.30 | C |
| ATOM | 325 | CG1 | ILE | A | 56 | 28.810 | 24.789 | 13.213 | 1.00 | 36.97 | C |
| ATOM | 326 | CG2 | ILE | A | 56 | 30.968 | 24.602 | 14.397 | 1.00 | 37.75 | C |
| ATOM | 327 | CD1 | ILE | A | 56 | 28.543 | 23.358 | 12.820 | 1.00 | 36.35 | C |
| ATOM | 328 | N | GLU | A | 57 | 32.627 | 26.899 | 12.204 | 1.00 | 37.67 | N |
| ATOM | 329 | CA | GLU | A | 57 | 34.045 | 27.204 | 12.166 | 1.00 | 38.21 | C |
| ATOM | 330 | C | GLU | A | 57 | 34.277 | 28.569 | 12.784 | 1.00 | 38.33 | C |
| ATOM | 331 | O | GLU | A | 57 | 35.210 | 28.758 | 13.566 | 1.00 | 38.33 | O |
| ATOM | 332 | CB | GLU | A | 57 | 34.547 | 27.214 | 10.725 | 1.00 | 38.49 | C |
| ATOM | 333 | CG | GLU | A | 57 | 36.038 | 27.461 | 10.559 | 1.00 | 40.09 | C |
| ATOM | 334 | CD | GLU | A | 57 | 36.870 | 26.539 | 11.424 | 1.00 | 42.96 | C |
| ATOM | 335 | OE1 | GLU | A | 57 | 36.527 | 25.329 | 11.487 | 1.00 | 43.20 | O |
| ATOM | 336 | OE2 | GLU | A | 57 | 37.852 | 27.032 | 12.044 | 1.00 | 44.14 | O |
| ATOM | 337 | N | ASN | A | 58 | 33.394 | 29.508 | 12.460 | 1.00 | 38.32 | N |
| ATOM | 338 | CA | ASN | A | 58 | 33.546 | 30.890 | 12.891 | 1.00 | 38.38 | C |
| ATOM | 339 | C | ASN | A | 58 | 32.849 | 31.221 | 14.167 | 1.00 | 38.06 | C |
| ATOM | 340 | O | ASN | A | 58 | 32.683 | 32.387 | 14.507 | 1.00 | 37.86 | O |
| ATOM | 341 | CB | ASN | A | 58 | 32.955 | 31.813 | 11.853 | 1.00 | 38.73 | C |
| ATOM | 342 | CG | ASN | A | 58 | 33.991 | 32.455 | 11.013 | 1.00 | 39.49 | C |
| ATOM | 343 | OD1 | ASN | A | 58 | 34.501 | 31.841 | 10.083 | 1.00 | 42.51 | O |
| ATOM | 344 | ND2 | ASN | A | 58 | 34.322 | 33.704 | 11.324 | 1.00 | 40.15 | N |
| ATOM | 345 | N | GLU | A | 59 | 32.399 | 30.196 | 14.856 | 1.00 | 37.88 | N |
| ATOM | 346 | CA | GLU | A | 59 | 31.683 | 30.396 | 16.092 | 1.00 | 37.68 | C |
| ATOM | 347 | C | GLU | A | 59 | 30.479 | 31.307 | 16.005 | 1.00 | 37.57 | C |
| ATOM | 348 | O | GLU | A | 59 | 30.305 | 32.203 | 16.813 | 1.00 | 36.94 | O |
| ATOM | 349 | CB | GLU | A | 59 | 32.663 | 30.857 | 17.118 | 1.00 | 37.60 | C |
| ATOM | 350 | CG | GLU | A | 59 | 33.710 | 29.785 | 17.212 | 1.00 | 38.25 | C |
| ATOM | 351 | CD | GLU | A | 59 | 34.545 | 29.886 | 18.435 | 1.00 | 38.10 | C |
| ATOM | 352 | OE1 | GLU | A | 59 | 35.654 | 30.430 | 18.303 | 1.00 | 40.30 | O |
| ATOM | 353 | OE2 | GLU | A | 59 | 34.089 | 29.420 | 19.498 | 1.00 | 37.62 | O |
| ATOM | 354 | N | GLU | A | 60 | 29.630 | 31.025 | 15.025 | 1.00 | 37.73 | N |
| ATOM | 355 | CA | GLU | A | 60 | 28.347 | 31.692 | 14.902 | 1.00 | 37.79 | C |
| ATOM | 356 | C | GLU | A | 60 | 27.290 | 30.620 | 14.923 | 1.00 | 37.12 | C |
| ATOM | 357 | O | GLU | A | 60 | 27.488 | 29.539 | 14.388 | 1.00 | 37.94 | O |
| ATOM | 358 | CB | GLU | A | 60 | 28.252 | 32.456 | 13.606 | 1.00 | 38.14 | C |
| ATOM | 359 | CG | GLU | A | 60 | 29.388 | 33.411 | 13.414 | 1.00 | 39.56 | C |
| ATOM | 360 | CD | GLU | A | 60 | 28.986 | 34.547 | 12.518 | 1.00 | 42.62 | C |
| ATOM | 361 | OE1 | GLU | A | 60 | 29.023 | 34.389 | 11.276 | 1.00 | 42.22 | O |
| ATOM | 362 | OE2 | GLU | A | 60 | 28.611 | 35.601 | 13.082 | 1.00 | 46.90 | O |
| ATOM | 363 | N | PRO | A | 61 | 26.158 | 30.917 | 15.517 | 1.00 | 36.25 | N |
| ATOM | 364 | CA | PRO | A | 61 | 25.111 | 29.919 | 15.680 | 1.00 | 36.11 | C |
| ATOM | 365 | C | PRO | A | 61 | 24.522 | 29.448 | 14.373 | 1.00 | 35.80 | C |
| ATOM | 366 | O | PRO | A | 61 | 24.534 | 30.159 | 13.386 | 1.00 | 36.29 | O |
| ATOM | 367 | CB | PRO | A | 61 | 24.021 | 30.672 | 16.442 | 1.00 | 36.35 | C |
| ATOM | 368 | CG | PRO | A | 61 | 24.367 | 32.117 | 16.353 | 1.00 | 36.05 | C |
| ATOM | 369 | CD | PRO | A | 61 | 25.790 | 32.228 | 16.061 | 1.00 | 36.10 | C |
| ATOM | 370 | N | VAL | A | 62 | 23.981 | 28.247 | 14.380 | 1.00 | 35.41 | N |
| ATOM | 371 | CA | VAL | A | 62 | 23.291 | 27.722 | 13.228 | 1.00 | 34.88 | C |
| ATOM | 372 | C | VAL | A | 62 | 22.438 | 26.584 | 13.720 | 1.00 | 34.68 | C |
| ATOM | 373 | O | VAL | A | 62 | 22.807 | 25.885 | 14.658 | 1.00 | 34.41 | O |
| ATOM | 374 | CB | VAL | A | 62 | 24.237 | 27.189 | 12.156 | 1.00 | 34.79 | C |
| ATOM | 375 | CG1 | VAL | A | 62 | 25.108 | 26.062 | 12.695 | 1.00 | 34.66 | C |
| ATOM | 376 | CG2 | VAL | A | 62 | 23.440 | 26.693 | 10.996 | 1.00 | 34.83 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 377 | N | VAL | A | 63 | 21.271 | 26.418 | 13.118 | 1.00 | 34.54 | N |
| ATOM | 378 | CA | VAL | A | 63 | 20.454 | 25.273 | 13.447 | 1.00 | 34.18 | C |
| ATOM | 379 | C | VAL | A | 63 | 20.660 | 24.230 | 12.372 | 1.00 | 33.85 | C |
| ATOM | 380 | O | VAL | A | 63 | 20.486 | 24.512 | 11.203 | 1.00 | 33.36 | O |
| ATOM | 381 | CB | VAL | A | 63 | 18.980 | 25.622 | 13.523 | 1.00 | 34.05 | C |
| ATOM | 382 | CG1 | VAL | A | 63 | 18.167 | 24.349 | 13.626 | 1.00 | 34.14 | C |
| ATOM | 383 | CG2 | VAL | A | 63 | 18.717 | 26.502 | 14.710 | 1.00 | 33.51 | C |
| ATOM | 384 | N | LEU | A | 64 | 21.048 | 23.028 | 12.769 | 1.00 | 33.87 | N |
| ATOM | 385 | CA | LEU | A | 64 | 21.204 | 21.942 | 11.814 | 1.00 | 34.03 | C |
| ATOM | 386 | C | LEU | A | 64 | 19.894 | 21.193 | 11.856 | 1.00 | 33.70 | C |
| ATOM | 387 | O | LEU | A | 64 | 19.368 | 20.956 | 12.932 | 1.00 | 34.18 | O |
| ATOM | 388 | CB | LEU | A | 64 | 22.417 | 21.071 | 12.164 | 1.00 | 33.90 | C |
| ATOM | 389 | CG | LEU | A | 64 | 23.667 | 21.978 | 12.155 | 1.00 | 34.85 | C |
| ATOM | 390 | CD1 | LEU | A | 64 | 24.975 | 21.303 | 12.485 | 1.00 | 35.82 | C |
| ATOM | 391 | CD2 | LEU | A | 64 | 23.821 | 22.629 | 10.798 | 1.00 | 35.39 | C |
| ATOM | 392 | N | THR | A | 65 | 19.314 | 20.887 | 10.704 | 1.00 | 33.36 | N |
| ATOM | 393 | CA | THR | A | 65 | 18.035 | 20.177 | 10.704 | 1.00 | 33.24 | C |
| ATOM | 394 | C | THR | A | 65 | 18.105 | 18.683 | 10.517 | 1.00 | 32.87 | C |
| ATOM | 395 | O | THR | A | 65 | 17.096 | 18.016 | 10.715 | 1.00 | 32.11 | O |
| ATOM | 396 | CB | THR | A | 65 | 17.149 | 20.657 | 9.562 | 1.00 | 33.35 | C |
| ATOM | 397 | OG1 | THR | A | 65 | 17.858 | 20.540 | 8.320 | 1.00 | 33.15 | O |
| ATOM | 398 | CG2 | THR | A | 65 | 16.843 | 22.093 | 9.693 | 1.00 | 33.51 | C |
| ATOM | 399 | N | ASP | A | 66 | 19.265 | 18.173 | 10.106 | 1.00 | 33.09 | N |
| ATOM | 400 | CA | ASP | A | 66 | 19.392 | 16.767 | 9.724 | 1.00 | 33.53 | C |
| ATOM | 401 | C | ASP | A | 66 | 20.629 | 16.019 | 10.189 | 1.00 | 33.55 | C |
| ATOM | 402 | O | ASP | A | 66 | 21.136 | 15.179 | 9.458 | 1.00 | 33.68 | O |
| ATOM | 403 | CB | ASP | A | 66 | 19.339 | 16.653 | 8.192 | 1.00 | 33.55 | C |
| ATOM | 404 | CG | ASP | A | 66 | 20.397 | 17.484 | 7.508 | 1.00 | 34.00 | C |
| ATOM | 405 | OD1 | ASP | A | 66 | 21.124 | 18.232 | 8.188 | 1.00 | 35.03 | O |
| ATOM | 406 | OD2 | ASP | A | 66 | 20.583 | 17.456 | 6.284 | 1.00 | 35.31 | O |
| ATOM | 407 | N | THR | A | 67 | 21.107 | 16.264 | 11.397 | 1.00 | 33.83 | N |
| ATOM | 408 | CA | THR | A | 67 | 22.286 | 15.540 | 11.845 | 1.00 | 33.70 | C |
| ATOM | 409 | C | THR | A | 67 | 21.937 | 14.177 | 12.340 | 1.00 | 33.84 | C |
| ATOM | 410 | O | THR | A | 67 | 22.808 | 13.340 | 12.431 | 1.00 | 34.42 | O |
| ATOM | 411 | CB | THR | A | 67 | 22.951 | 16.215 | 13.020 | 1.00 | 33.66 | C |
| ATOM | 412 | OG1 | THR | A | 67 | 21.981 | 16.451 | 14.046 | 1.00 | 33.90 | O |
| ATOM | 413 | CG2 | THR | A | 67 | 23.472 | 17.562 | 12.674 | 1.00 | 33.56 | C |
| ATOM | 414 | N | ASN | A | 68 | 20.686 | 13.954 | 12.719 | 1.00 | 34.00 | N |
| ATOM | 415 | CA | ASN | A | 68 | 20.320 | 12.676 | 13.312 | 1.00 | 34.15 | C |
| ATOM | 416 | C | ASN | A | 68 | 21.108 | 12.454 | 14.575 | 1.00 | 33.97 | C |
| ATOM | 417 | O | ASN | A | 68 | 21.281 | 11.330 | 15.008 | 1.00 | 33.83 | O |
| ATOM | 418 | CB | ASN | A | 68 | 20.653 | 11.531 | 12.375 | 1.00 | 34.26 | C |
| ATOM | 419 | CG | ASN | A | 68 | 19.685 | 11.411 | 11.239 | 1.00 | 35.12 | C |
| ATOM | 420 | OD1 | ASN | A | 68 | 18.512 | 11.104 | 11.434 | 1.00 | 35.89 | O |
| ATOM | 421 | ND2 | ASN | A | 68 | 20.168 | 11.649 | 10.033 | 1.00 | 36.88 | N |
| ATOM | 422 | N | LEU | A | 69 | 21.598 | 13.531 | 15.162 | 1.00 | 34.12 | N |
| ATOM | 423 | CA | LEU | A | 69 | 22.446 | 13.419 | 16.334 | 1.00 | 34.19 | C |
| ATOM | 424 | C | LEU | A | 69 | 21.836 | 12.562 | 17.440 | 1.00 | 34.16 | C |
| ATOM | 425 | O | LEU | A | 69 | 22.538 | 11.737 | 18.039 | 1.00 | 33.75 | O |
| ATOM | 426 | CB | LEU | A | 69 | 22.774 | 14.808 | 16.881 | 1.00 | 34.13 | C |
| ATOM | 427 | CG | LEU | A | 69 | 23.652 | 14.795 | 18.125 | 1.00 | 34.10 | C |
| ATOM | 428 | CD1 | LEU | A | 69 | 24.978 | 14.105 | 17.854 | 1.00 | 34.66 | C |
| ATOM | 429 | CD2 | LEU | A | 69 | 23.883 | 16.183 | 18.582 | 1.00 | 33.94 | C |
| ATOM | 430 | N | VAL | A | 70 | 20.555 | 12.783 | 17.732 | 1.00 | 34.15 | N |
| ATOM | 431 | CA | VAL | A | 70 | 19.877 | 12.023 | 18.777 | 1.00 | 34.48 | C |
| ATOM | 432 | C | VAL | A | 70 | 18.654 | 11.307 | 18.228 | 1.00 | 34.64 | C |
| ATOM | 433 | O | VAL | A | 70 | 17.600 | 11.223 | 18.865 | 1.00 | 34.46 | O |
| ATOM | 434 | CB | VAL | A | 70 | 19.540 | 12.899 | 20.003 | 1.00 | 34.61 | C |
| ATOM | 435 | CG1 | VAL | A | 70 | 20.808 | 13.555 | 20.519 | 1.00 | 35.04 | C |
| ATOM | 436 | CG2 | VAL | A | 70 | 18.493 | 13.939 | 19.706 | 1.00 | 34.21 | C |
| ATOM | 437 | N | TYR | A | 71 | 18.833 | 10.762 | 17.033 | 1.00 | 34.98 | N |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 438 | CA | TYR | A | 71 | 17.779 | 10.041 | 16.352 | 1.00 | 35.19 | C |
| ATOM | 439 | C | TYR | A | 71 | 17.051 | 9.086 | 17.305 | 1.00 | 35.24 | C |
| ATOM | 440 | O | TYR | A | 71 | 15.837 | 9.148 | 17.421 | 1.00 | 35.61 | O |
| ATOM | 441 | CB | TYR | A | 71 | 18.337 | 9.291 | 15.137 | 1.00 | 35.26 | C |
| ATOM | 442 | CG | TYR | A | 71 | 17.352 | 8.278 | 14.618 | 1.00 | 35.95 | C |
| ATOM | 443 | CD1 | TYR | A | 71 | 16.155 | 8.696 | 14.055 | 1.00 | 35.96 | C |
| ATOM | 444 | CD2 | TYR | A | 71 | 17.584 | 6.915 | 14.731 | 1.00 | 34.66 | C |
| ATOM | 445 | CE1 | TYR | A | 71 | 15.239 | 7.805 | 13.610 | 1.00 | 35.86 | C |
| ATOM | 446 | CE2 | TYR | A | 71 | 16.664 | 6.011 | 14.281 | 1.00 | 34.47 | C |
| ATOM | 447 | CZ | TYR | A | 71 | 15.485 | 6.463 | 13.724 | 1.00 | 36.06 | C |
| ATOM | 448 | OH | TYR | A | 71 | 14.518 | 5.589 | 13.248 | 1.00 | 38.92 | O |
| ATOM | 449 | N | PRO | A | 72 | 17.774 | 8.211 | 17.993 | 1.00 | 35.15 | N |
| ATOM | 450 | CA | PRO | A | 72 | 17.141 | 7.271 | 18.924 | 1.00 | 35.16 | C |
| ATOM | 451 | C | PRO | A | 72 | 16.357 | 7.923 | 20.068 | 1.00 | 35.14 | C |
| ATOM | 452 | O | PRO | A | 72 | 15.473 | 7.294 | 20.643 | 1.00 | 34.97 | O |
| ATOM | 453 | CB | PRO | A | 72 | 18.327 | 6.475 | 19.487 | 1.00 | 35.18 | C |
| ATOM | 454 | CG | PRO | A | 72 | 19.433 | 6.677 | 18.524 | 1.00 | 35.26 | C |
| ATOM | 455 | CD | PRO | A | 72 | 19.233 | 8.031 | 17.938 | 1.00 | 35.29 | C |
| ATOM | 456 | N | ALA | A | 73 | 16.657 | 9.169 | 20.401 | 1.00 | 35.18 | N |
| ATOM | 457 | CA | ALA | A | 73 | 15.967 | 9.803 | 21.512 | 1.00 | 35.21 | C |
| ATOM | 458 | C | ALA | A | 73 | 14.657 | 10.414 | 21.097 | 1.00 | 35.08 | C |
| ATOM | 459 | O | ALA | A | 73 | 13.890 | 10.862 | 21.934 | 1.00 | 34.86 | O |
| ATOM | 460 | CB | ALA | A | 73 | 16.829 | 10.864 | 22.135 | 1.00 | 35.37 | C |
| ATOM | 461 | N | LEU | A | 74 | 14.370 | 10.434 | 19.812 | 1.00 | 35.25 | N |
| ATOM | 462 | CA | LEU | A | 74 | 13.142 | 11.090 | 19.399 | 1.00 | 35.54 | C |
| ATOM | 463 | C | LEU | A | 74 | 11.903 | 10.434 | 19.958 | 1.00 | 35.66 | C |
| ATOM | 464 | O | LEU | A | 74 | 10.893 | 11.088 | 20.118 | 1.00 | 35.64 | O |
| ATOM | 465 | CB | LEU | A | 74 | 13.044 | 11.190 | 17.894 | 1.00 | 35.31 | C |
| ATOM | 466 | CG | LEU | A | 74 | 14.161 | 12.046 | 17.333 | 1.00 | 36.48 | C |
| ATOM | 467 | CD1 | LEU | A | 74 | 13.887 | 12.277 | 15.890 | 1.00 | 37.76 | C |
| ATOM | 468 | CD2 | LEU | A | 74 | 14.300 | 13.394 | 18.076 | 1.00 | 37.06 | C |
| ATOM | 469 | N | LYS | A | 75 | 11.979 | 9.151 | 20.282 | 1.00 | 36.19 | N |
| ATOM | 470 | CA | LYS | A | 75 | 10.795 | 8.453 | 20.767 | 1.00 | 36.36 | C |
| ATOM | 471 | C | LYS | A | 75 | 10.566 | 8.710 | 22.246 | 1.00 | 36.85 | C |
| ATOM | 472 | O | LYS | A | 75 | 9.491 | 8.437 | 22.765 | 1.00 | 37.12 | O |
| ATOM | 473 | CB | LYS | A | 75 | 10.904 | 6.956 | 20.505 | 1.00 | 36.04 | C |
| ATOM | 474 | CG | LYS | A | 75 | 12.060 | 6.284 | 21.216 | 1.00 | 35.77 | C |
| ATOM | 475 | CD | LYS | A | 75 | 12.245 | 4.829 | 20.782 | 1.00 | 34.46 | C |
| ATOM | 476 | CE | LYS | A | 75 | 13.720 | 4.460 | 20.710 | 1.00 | 33.42 | C |
| ATOM | 477 | NZ | LYS | A | 75 | 14.375 | 4.536 | 22.036 | 1.00 | 32.34 | N |
| ATOM | 478 | N | TRP | A | 76 | 11.578 | 9.244 | 22.920 | 1.00 | 37.24 | N |
| ATOM | 479 | CA | TRP | A | 76 | 11.481 | 9.510 | 24.345 | 1.00 | 37.30 | C |
| ATOM | 480 | C | TRP | A | 76 | 10.274 | 10.369 | 24.700 | 1.00 | 37.42 | C |
| ATOM | 481 | O | TRP | A | 76 | 9.917 | 11.306 | 23.984 | 1.00 | 37.54 | O |
| ATOM | 482 | CB | TRP | A | 76 | 12.728 | 10.247 | 24.838 | 1.00 | 37.12 | C |
| ATOM | 483 | CG | TRP | A | 76 | 13.980 | 9.446 | 24.816 | 1.00 | 36.77 | C |
| ATOM | 484 | CD1 | TRP | A | 76 | 14.142 | 8.176 | 24.359 | 1.00 | 37.03 | C |
| ATOM | 485 | CD2 | TRP | A | 76 | 15.255 | 9.864 | 25.291 | 1.00 | 36.31 | C |
| ATOM | 486 | NE1 | TRP | A | 76 | 15.445 | 7.776 | 24.527 | 1.00 | 36.52 | N |
| ATOM | 487 | CE2 | TRP | A | 76 | 16.147 | 8.801 | 25.097 | 1.00 | 36.08 | C |
| ATOM | 488 | CE3 | TRP | A | 76 | 15.737 | 11.040 | 25.864 | 1.00 | 36.23 | C |
| ATOM | 489 | CZ2 | TRP | A | 76 | 17.480 | 8.881 | 25.443 | 1.00 | 36.27 | C |
| ATOM | 490 | CZ3 | TRP | A | 76 | 17.055 | 11.113 | 26.209 | 1.00 | 36.35 | C |
| ATOM | 491 | CH2 | TRP | A | 76 | 17.915 | 10.045 | 25.996 | 1.00 | 36.41 | C |
| ATOM | 492 | N | ASP | A | 77 | 9.662 | 10.015 | 25.820 | 1.00 | 37.42 | N |
| ATOM | 493 | CA | ASP | A | 77 | 8.591 | 10.768 | 26.435 | 1.00 | 37.36 | C |
| ATOM | 494 | C | ASP | A | 77 | 8.707 | 10.370 | 27.907 | 1.00 | 37.09 | C |
| ATOM | 495 | O | ASP | A | 77 | 9.628 | 9.647 | 28.260 | 1.00 | 37.04 | O |
| ATOM | 496 | CB | ASP | A | 77 | 7.245 | 10.377 | 25.834 | 1.00 | 37.48 | C |
| ATOM | 497 | CG | ASP | A | 77 | 6.990 | 8.888 | 25.903 | 1.00 | 38.01 | C |
| ATOM | 498 | OD1 | ASP | A | 77 | 7.704 | 8.191 | 26.658 | 1.00 | 38.42 | O |

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ATOM    499  OD2 ASP A  77       6.093   8.319  25.244  1.00 39.67           O
ATOM    500  N   LEU A  78       7.789  10.798  28.763  1.00 36.79           N
ATOM    501  CA  LEU A  78       7.913  10.496  30.182  1.00 36.49           C
ATOM    502  C   LEU A  78       7.729   9.026  30.464  1.00 36.62           C
ATOM    503  O   LEU A  78       8.456   8.426  31.260  1.00 36.50           O
ATOM    504  CB  LEU A  78       6.903  11.296  30.974  1.00 36.33           C
ATOM    505  CG  LEU A  78       7.119  12.796  30.863  1.00 36.49           C
ATOM    506  CD1 LEU A  78       6.008  13.510  31.594  1.00 36.63           C
ATOM    507  CD2 LEU A  78       8.494  13.194  31.399  1.00 36.10           C
ATOM    508  N   GLU A  79       6.748   8.433  29.815  1.00 36.81           N
ATOM    509  CA  GLU A  79       6.505   7.030  30.041  1.00 36.97           C
ATOM    510  C   GLU A  79       7.737   6.176  29.738  1.00 36.75           C
ATOM    511  O   GLU A  79       8.151   5.373  30.572  1.00 36.84           O
ATOM    512  CB  GLU A  79       5.323   6.560  29.214  1.00 37.25           C
ATOM    513  CG  GLU A  79       4.937   5.137  29.540  1.00 37.93           C
ATOM    514  CD  GLU A  79       3.729   4.681  28.768  1.00 38.61           C
ATOM    515  OE1 GLU A  79       3.381   5.352  27.775  1.00 38.32           O
ATOM    516  OE2 GLU A  79       3.131   3.654  29.166  1.00 40.10           O
ATOM    517  N   TYR A  80       8.318   6.337  28.553  1.00 36.50           N
ATOM    518  CA  TYR A  80       9.489   5.549  28.176  1.00 36.32           C
ATOM    519  C   TYR A  80      10.644   5.804  29.123  1.00 36.27           C
ATOM    520  O   TYR A  80      11.343   4.872  29.516  1.00 36.15           O
ATOM    521  CB  TYR A  80       9.921   5.889  26.751  1.00 36.39           C
ATOM    522  CG  TYR A  80      11.180   5.202  26.228  1.00 36.06           C
ATOM    523  CD1 TYR A  80      11.100   4.000  25.557  1.00 36.22           C
ATOM    524  CD2 TYR A  80      12.432   5.793  26.349  1.00 35.91           C
ATOM    525  CE1 TYR A  80      12.225   3.380  25.051  1.00 36.52           C
ATOM    526  CE2 TYR A  80      13.568   5.179  25.844  1.00 36.04           C
ATOM    527  CZ  TYR A  80      13.454   3.967  25.190  1.00 36.46           C
ATOM    528  OH  TYR A  80      14.561   3.321  24.673  1.00 35.81           O
ATOM    529  N   LEU A  81      10.846   7.064  29.493  1.00 36.13           N
ATOM    530  CA  LEU A  81      11.971   7.408  30.353  1.00 36.22           C
ATOM    531  C   LEU A  81      11.777   6.827  31.747  1.00 36.13           C
ATOM    532  O   LEU A  81      12.706   6.259  32.325  1.00 35.90           O
ATOM    533  CB  LEU A  81      12.208   8.930  30.406  1.00 36.22           C
ATOM    534  CG  LEU A  81      12.774   9.568  29.121  1.00 36.35           C
ATOM    535  CD1 LEU A  81      12.880  11.055  29.274  1.00 36.49           C
ATOM    536  CD2 LEU A  81      14.132   9.017  28.718  1.00 36.18           C
ATOM    537  N   GLN A  82      10.569   6.956  32.280  1.00 36.15           N
ATOM    538  CA  GLN A  82      10.284   6.424  33.597  1.00 36.29           C
ATOM    539  C   GLN A  82      10.575   4.927  33.605  1.00 36.25           C
ATOM    540  O   GLN A  82      11.210   4.408  34.515  1.00 35.96           O
ATOM    541  CB  GLN A  82       8.838   6.710  33.976  1.00 36.38           C
ATOM    542  CG  GLN A  82       8.418   6.080  35.279  1.00 37.00           C
ATOM    543  CD  GLN A  82       7.191   6.740  35.872  1.00 37.85           C
ATOM    544  OE1 GLN A  82       6.640   7.676  35.295  1.00 38.24           O
ATOM    545  NE2 GLN A  82       6.754   6.247  37.020  1.00 38.93           N
ATOM    546  N   GLU A  83      10.136   4.240  32.560  1.00 36.46           N
ATOM    547  CA  GLU A  83      10.366   2.807  32.451  1.00 36.59           C
ATOM    548  C   GLU A  83      11.843   2.424  32.307  1.00 36.50           C
ATOM    549  O   GLU A  83      12.228   1.321  32.677  1.00 36.55           O
ATOM    550  CB  GLU A  83       9.568   2.237  31.271  1.00 36.57           C
ATOM    551  CG  GLU A  83       9.497   0.714  31.239  1.00 36.95           C
ATOM    552  CD  GLU A  83       8.732   0.107  32.416  1.00 37.61           C
ATOM    553  OE1 GLU A  83       7.922   0.815  33.050  1.00 37.88           O
ATOM    554  OE2 GLU A  83       8.938  -1.090  32.719  1.00 37.54           O
ATOM    555  N   ASN A  84      12.680   3.324  31.805  1.00 36.58           N
ATOM    556  CA  ASN A  84      14.049   2.936  31.476  1.00 36.62           C
ATOM    557  C   ASN A  84      15.210   3.749  32.001  1.00 36.66           C
ATOM    558  O   ASN A  84      16.349   3.310  31.900  1.00 36.62           O
ATOM    559  CB  ASN A  84      14.211   2.936  29.960  1.00 36.62           C
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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 560 | CG | ASN | A | 84 | 13.362 | 1.902 | 29.286 | 1.00 | 36.37 | C |
| ATOM | 561 | OD1 | ASN | A | 84 | 13.352 | 0.733 | 29.683 | 1.00 | 36.46 | O |
| ATOM | 562 | ND2 | ASN | A | 84 | 12.644 | 2.317 | 28.247 | 1.00 | 35.65 | N |
| ATOM | 563 | N | ILE | A | 85 | 14.975 | 4.920 | 32.557 | 1.00 | 36.80 | N |
| ATOM | 564 | CA | ILE | A | 85 | 16.125 | 5.730 | 32.885 | 1.00 | 37.13 | C |
| ATOM | 565 | C | ILE | A | 85 | 16.834 | 5.365 | 34.180 | 1.00 | 37.28 | C |
| ATOM | 566 | O | ILE | A | 85 | 17.793 | 6.022 | 34.568 | 1.00 | 37.74 | O |
| ATOM | 567 | CB | ILE | A | 85 | 15.752 | 7.184 | 32.874 | 1.00 | 37.21 | C |
| ATOM | 568 | CG1 | ILE | A | 85 | 16.958 | 8.009 | 32.445 | 1.00 | 37.55 | C |
| ATOM | 569 | CG2 | ILE | A | 85 | 15.241 | 7.593 | 34.222 | 1.00 | 37.38 | C |
| ATOM | 570 | CD1 | ILE | A | 85 | 16.623 | 9.467 | 32.195 | 1.00 | 37.68 | C |
| ATOM | 571 | N | GLY | A | 86 | 16.383 | 4.326 | 34.855 | 1.00 | 37.29 | N |
| ATOM | 572 | CA | GLY | A | 86 | 17.089 | 3.892 | 36.038 | 1.00 | 37.39 | C |
| ATOM | 573 | C | GLY | A | 86 | 16.553 | 4.496 | 37.308 | 1.00 | 37.43 | C |
| ATOM | 574 | O | GLY | A | 86 | 15.583 | 5.265 | 37.290 | 1.00 | 37.34 | O |
| ATOM | 575 | N | ASN | A | 87 | 17.212 | 4.167 | 38.414 | 1.00 | 37.34 | N |
| ATOM | 576 | CA | ASN | A | 87 | 16.750 | 4.602 | 39.716 | 1.00 | 37.42 | C |
| ATOM | 577 | C | ASN | A | 87 | 17.701 | 5.603 | 40.357 | 1.00 | 37.39 | C |
| ATOM | 578 | O | ASN | A | 87 | 17.740 | 5.742 | 41.578 | 1.00 | 37.39 | O |
| ATOM | 579 | CB | ASN | A | 87 | 16.545 | 3.399 | 40.612 | 1.00 | 37.40 | C |
| ATOM | 580 | N | GLY | A | 88 | 18.451 | 6.321 | 39.529 | 1.00 | 37.47 | N |
| ATOM | 581 | CA | GLY | A | 88 | 19.405 | 7.296 | 40.028 | 1.00 | 37.41 | C |
| ATOM | 582 | C | GLY | A | 88 | 18.686 | 8.554 | 40.450 | 1.00 | 37.30 | C |
| ATOM | 583 | O | GLY | A | 88 | 17.500 | 8.709 | 40.171 | 1.00 | 37.36 | O |
| ATOM | 584 | N | ASP | A | 89 | 19.390 | 9.453 | 41.125 | 1.00 | 37.26 | N |
| ATOM | 585 | CA | ASP | A | 89 | 18.780 | 10.716 | 41.531 | 1.00 | 37.21 | C |
| ATOM | 586 | C | ASP | A | 89 | 18.726 | 11.681 | 40.355 | 1.00 | 36.91 | C |
| ATOM | 587 | O | ASP | A | 89 | 19.607 | 11.654 | 39.500 | 1.00 | 36.62 | O |
| ATOM | 588 | CB | ASP | A | 89 | 19.563 | 11.346 | 42.680 | 1.00 | 37.24 | C |
| ATOM | 589 | CG | ASP | A | 89 | 19.277 | 10.690 | 44.000 | 1.00 | 37.24 | C |
| ATOM | 590 | OD1 | ASP | A | 89 | 18.398 | 9.802 | 44.044 | 1.00 | 37.14 | O |
| ATOM | 591 | OD2 | ASP | A | 89 | 19.876 | 11.002 | 45.047 | 1.00 | 37.98 | O |
| ATOM | 592 | N | PHE | A | 90 | 17.667 | 12.492 | 40.295 | 1.00 | 36.88 | N |
| ATOM | 593 | CA | PHE | A | 90 | 17.554 | 13.570 | 39.298 | 1.00 | 36.87 | C |
| ATOM | 594 | C | PHE | A | 90 | 17.327 | 14.926 | 39.942 | 1.00 | 36.79 | C |
| ATOM | 595 | O | PHE | A | 90 | 16.455 | 15.080 | 40.795 | 1.00 | 36.69 | O |
| ATOM | 596 | CB | PHE | A | 90 | 16.420 | 13.308 | 38.321 | 1.00 | 36.70 | C |
| ATOM | 597 | CG | PHE | A | 90 | 16.712 | 12.210 | 37.371 | 1.00 | 36.83 | C |
| ATOM | 598 | CD1 | PHE | A | 90 | 16.551 | 10.901 | 37.757 | 1.00 | 36.07 | C |
| ATOM | 599 | CD2 | PHE | A | 90 | 17.191 | 12.479 | 36.102 | 1.00 | 37.27 | C |
| ATOM | 600 | CE1 | PHE | A | 90 | 16.827 | 9.885 | 36.899 | 1.00 | 35.81 | C |
| ATOM | 601 | CE2 | PHE | A | 90 | 17.475 | 11.449 | 35.238 | 1.00 | 36.82 | C |
| ATOM | 602 | CZ | PHE | A | 90 | 17.291 | 10.150 | 35.642 | 1.00 | 36.06 | C |
| ATOM | 603 | N | SER | A | 91 | 18.123 | 15.905 | 39.529 | 1.00 | 36.92 | N |
| ATOM | 604 | CA | SER | A | 91 | 17.971 | 17.266 | 40.027 | 1.00 | 36.99 | C |
| ATOM | 605 | C | SER | A | 91 | 16.738 | 17.923 | 39.428 | 1.00 | 37.10 | C |
| ATOM | 606 | O | SER | A | 91 | 16.586 | 17.985 | 38.206 | 1.00 | 36.78 | O |
| ATOM | 607 | CB | SER | A | 91 | 19.200 | 18.105 | 39.699 | 1.00 | 36.86 | C |
| ATOM | 608 | OG | SER | A | 91 | 20.350 | 17.616 | 40.358 | 1.00 | 36.54 | O |
| ATOM | 609 | N | VAL | A | 92 | 15.857 | 18.402 | 40.303 | 1.00 | 37.42 | N |
| ATOM | 610 | CA | VAL | A | 92 | 14.660 | 19.106 | 39.876 | 1.00 | 37.75 | C |
| ATOM | 611 | C | VAL | A | 92 | 14.509 | 20.468 | 40.545 | 1.00 | 38.10 | C |
| ATOM | 612 | O | VAL | A | 92 | 14.472 | 20.589 | 41.768 | 1.00 | 38.08 | O |
| ATOM | 613 | CB | VAL | A | 92 | 13.406 | 18.303 | 40.159 | 1.00 | 37.63 | C |
| ATOM | 614 | CG1 | VAL | A | 92 | 12.197 | 19.034 | 39.621 | 1.00 | 37.42 | C |
| ATOM | 615 | CG2 | VAL | A | 92 | 13.515 | 16.946 | 39.527 | 1.00 | 37.78 | C |
| ATOM | 616 | N | TYR | A | 93 | 14.384 | 21.487 | 39.709 | 1.00 | 38.59 | N |
| ATOM | 617 | CA | TYR | A | 93 | 14.220 | 22.849 | 40.166 | 1.00 | 38.91 | C |
| ATOM | 618 | C | TYR | A | 93 | 12.784 | 23.173 | 40.219 | 1.00 | 39.41 | C |
| ATOM | 619 | O | TYR | A | 93 | 12.019 | 22.786 | 39.343 | 1.00 | 39.64 | O |
| ATOM | 620 | CB | TYR | A | 93 | 14.883 | 23.799 | 39.202 | 1.00 | 38.84 | C |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 621 | CG | TYR | A | 93 | 16.332 | 23.588 | 39.288 | 1.00 | 38.25 | C |
| ATOM | 622 | CD1 | TYR | A | 93 | 17.044 | 24.122 | 40.334 | 1.00 | 38.21 | C |
| ATOM | 623 | CD2 | TYR | A | 93 | 16.968 | 22.750 | 38.415 | 1.00 | 37.50 | C |
| ATOM | 624 | CE1 | TYR | A | 93 | 18.362 | 23.893 | 40.464 | 1.00 | 37.90 | C |
| ATOM | 625 | CE2 | TYR | A | 93 | 18.287 | 22.512 | 38.534 | 1.00 | 37.82 | C |
| ATOM | 626 | CZ | TYR | A | 93 | 18.987 | 23.090 | 39.557 | 1.00 | 37.78 | C |
| ATOM | 627 | OH | TYR | A | 93 | 20.322 | 22.836 | 39.677 | 1.00 | 39.39 | O |
| ATOM | 628 | N | SER | A | 94 | 12.422 | 23.935 | 41.228 | 1.00 | 40.00 | N |
| ATOM | 629 | CA | SER | A | 94 | 11.043 | 24.274 | 41.416 | 1.00 | 40.51 | C |
| ATOM | 630 | C | SER | A | 94 | 11.020 | 25.773 | 41.426 | 1.00 | 40.68 | C |
| ATOM | 631 | O | SER | A | 94 | 11.962 | 26.384 | 41.896 | 1.00 | 41.00 | O |
| ATOM | 632 | CB | SER | A | 94 | 10.539 | 23.693 | 42.730 | 1.00 | 40.58 | C |
| ATOM | 633 | OG | SER | A | 94 | 9.139 | 23.874 | 42.858 | 1.00 | 41.30 | O |
| ATOM | 634 | N | ALA | A | 95 | 9.974 | 26.374 | 40.878 | 1.00 | 40.87 | N |
| ATOM | 635 | CA | ALA | A | 95 | 9.899 | 27.824 | 40.856 | 1.00 | 40.91 | C |
| ATOM | 636 | C | ALA | A | 95 | 8.483 | 28.343 | 40.826 | 1.00 | 41.03 | C |
| ATOM | 637 | O | ALA | A | 95 | 7.573 | 27.699 | 40.309 | 1.00 | 41.09 | O |
| ATOM | 638 | CB | ALA | A | 95 | 10.630 | 28.350 | 39.668 | 1.00 | 40.93 | C |
| ATOM | 639 | N | SER | A | 96 | 8.328 | 29.549 | 41.350 | 1.00 | 41.12 | N |
| ATOM | 640 | CA | SER | A | 96 | 7.034 | 30.200 | 41.413 | 1.00 | 41.05 | C |
| ATOM | 641 | C | SER | A | 96 | 6.834 | 31.208 | 40.305 | 1.00 | 40.72 | C |
| ATOM | 642 | O | SER | A | 96 | 5.833 | 31.912 | 40.277 | 1.00 | 40.86 | O |
| ATOM | 643 | CB | SER | A | 96 | 6.902 | 30.938 | 42.731 | 1.00 | 41.16 | C |
| ATOM | 644 | OG | SER | A | 96 | 5.767 | 31.779 | 42.693 | 1.00 | 41.90 | O |
| ATOM | 645 | N | THR | A | 97 | 7.808 | 31.314 | 39.423 | 1.00 | 40.34 | N |
| ATOM | 646 | CA | THR | A | 97 | 7.710 | 32.209 | 38.292 | 1.00 | 40.18 | C |
| ATOM | 647 | C | THR | A | 97 | 8.073 | 31.368 | 37.113 | 1.00 | 39.72 | C |
| ATOM | 648 | O | THR | A | 97 | 8.582 | 30.274 | 37.279 | 1.00 | 39.83 | O |
| ATOM | 649 | CB | THR | A | 97 | 8.732 | 33.336 | 38.393 | 1.00 | 40.49 | C |
| ATOM | 650 | OG1 | THR | A | 97 | 8.905 | 33.946 | 37.105 | 1.00 | 41.00 | O |
| ATOM | 651 | CG2 | THR | A | 97 | 10.145 | 32.779 | 38.718 | 1.00 | 40.86 | C |
| ATOM | 652 | N | HIS | A | 98 | 7.862 | 31.874 | 35.915 | 1.00 | 39.32 | N |
| ATOM | 653 | CA | HIS | A | 98 | 8.257 | 31.112 | 34.754 | 1.00 | 39.12 | C |
| ATOM | 654 | C | HIS | A | 98 | 9.765 | 31.163 | 34.543 | 1.00 | 39.41 | C |
| ATOM | 655 | O | HIS | A | 98 | 10.299 | 30.423 | 33.711 | 1.00 | 39.15 | O |
| ATOM | 656 | CB | HIS | A | 98 | 7.576 | 31.646 | 33.516 | 1.00 | 38.95 | C |
| ATOM | 657 | CG | HIS | A | 98 | 7.807 | 33.104 | 33.290 | 1.00 | 38.64 | C |
| ATOM | 658 | ND1 | HIS | A | 98 | 7.095 | 34.081 | 33.950 | 1.00 | 37.36 | N |
| ATOM | 659 | CD2 | HIS | A | 98 | 8.672 | 33.753 | 32.477 | 1.00 | 38.57 | C |
| ATOM | 660 | CE1 | HIS | A | 98 | 7.509 | 35.268 | 33.550 | 1.00 | 37.33 | C |
| ATOM | 661 | NE2 | HIS | A | 98 | 8.463 | 35.098 | 32.654 | 1.00 | 37.37 | N |
| ATOM | 662 | N | LYS | A | 99 | 10.452 | 32.021 | 35.294 | 1.00 | 39.52 | N |
| ATOM | 663 | CA | LYS | A | 99 | 11.881 | 32.184 | 35.105 | 1.00 | 39.98 | C |
| ATOM | 664 | C | LYS | A | 99 | 12.749 | 31.364 | 36.029 | 1.00 | 40.38 | C |
| ATOM | 665 | O | LYS | A | 99 | 12.744 | 31.554 | 37.246 | 1.00 | 40.33 | O |
| ATOM | 666 | CB | LYS | A | 99 | 12.281 | 33.631 | 35.297 | 1.00 | 40.10 | C |
| ATOM | 667 | CG | LYS | A | 99 | 11.814 | 34.527 | 34.219 | 1.00 | 40.15 | C |
| ATOM | 668 | CD | LYS | A | 99 | 12.537 | 35.820 | 34.337 | 1.00 | 40.36 | C |
| ATOM | 669 | CE | LYS | A | 99 | 11.725 | 36.835 | 35.072 | 1.00 | 41.10 | C |
| ATOM | 670 | NZ | LYS | A | 99 | 10.975 | 37.655 | 34.074 | 1.00 | 41.52 | N |
| ATOM | 671 | N | PHE | A | 100 | 13.541 | 30.486 | 35.433 | 1.00 | 40.77 | N |
| ATOM | 672 | CA | PHE | A | 100 | 14.450 | 29.665 | 36.201 | 1.00 | 41.12 | C |
| ATOM | 673 | C | PHE | A | 100 | 15.893 | 30.159 | 36.218 | 1.00 | 41.78 | C |
| ATOM | 674 | O | PHE | A | 100 | 16.808 | 29.463 | 35.765 | 1.00 | 42.13 | O |
| ATOM | 675 | CB | PHE | A | 100 | 14.418 | 28.255 | 35.658 | 1.00 | 40.86 | C |
| ATOM | 676 | CG | PHE | A | 100 | 13.211 | 27.494 | 36.060 | 1.00 | 40.53 | C |
| ATOM | 677 | CD1 | PHE | A | 100 | 12.040 | 27.604 | 35.344 | 1.00 | 39.76 | C |
| ATOM | 678 | CD2 | PHE | A | 100 | 13.249 | 26.666 | 37.159 | 1.00 | 39.54 | C |
| ATOM | 679 | CE1 | PHE | A | 100 | 10.942 | 26.890 | 35.707 | 1.00 | 39.56 | C |
| ATOM | 680 | CE2 | PHE | A | 100 | 12.155 | 25.955 | 37.526 | 1.00 | 39.79 | C |
| ATOM | 681 | CZ | PHE | A | 100 | 10.995 | 26.064 | 36.802 | 1.00 | 39.91 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 682 | N | LEU | A | 101 | 16.124 | 31.347 | 36.747 | 1.00 | 42.23 | N |
| ATOM | 683 | CA | LEU | A | 101 | 17.501 | 31.800 | 36.868 | 1.00 | 42.74 | C |
| ATOM | 684 | C | LEU | A | 101 | 18.429 | 30.780 | 37.567 | 1.00 | 43.27 | C |
| ATOM | 685 | O | LEU | A | 101 | 18.213 | 30.392 | 38.736 | 1.00 | 43.22 | O |
| ATOM | 686 | CB | LEU | A | 101 | 17.549 | 33.097 | 37.657 | 1.00 | 42.90 | C |
| ATOM | 687 | CG | LEU | A | 101 | 18.900 | 33.800 | 37.793 | 1.00 | 43.35 | C |
| ATOM | 688 | CD1 | LEU | A | 101 | 19.441 | 34.288 | 36.455 | 1.00 | 43.59 | C |
| ATOM | 689 | CD2 | LEU | A | 101 | 18.703 | 34.967 | 38.724 | 1.00 | 43.91 | C |
| ATOM | 690 | N | TYR | A | 102 | 19.470 | 30.379 | 36.836 | 1.00 | 43.59 | N |
| ATOM | 691 | CA | TYR | A | 102 | 20.547 | 29.522 | 37.340 | 1.00 | 43.71 | C |
| ATOM | 692 | C | TYR | A | 102 | 21.380 | 30.186 | 38.460 | 1.00 | 43.57 | C |
| ATOM | 693 | O | TYR | A | 102 | 21.746 | 31.364 | 38.343 | 1.00 | 44.09 | O |
| ATOM | 694 | CB | TYR | A | 102 | 21.531 | 29.218 | 36.193 | 1.00 | 43.90 | C |
| ATOM | 695 | CG | TYR | A | 102 | 22.703 | 28.421 | 36.700 | 1.00 | 44.68 | C |
| ATOM | 696 | CD1 | TYR | A | 102 | 22.553 | 27.080 | 37.033 | 1.00 | 44.29 | C |
| ATOM | 697 | CD2 | TYR | A | 102 | 23.935 | 29.023 | 36.918 | 1.00 | 44.88 | C |
| ATOM | 698 | CE1 | TYR | A | 102 | 23.602 | 26.358 | 37.541 | 1.00 | 44.98 | C |
| ATOM | 699 | CE2 | TYR | A | 102 | 24.987 | 28.309 | 37.422 | 1.00 | 45.44 | C |
| ATOM | 700 | CZ | TYR | A | 102 | 24.826 | 26.984 | 37.735 | 1.00 | 45.86 | C |
| ATOM | 701 | OH | TYR | A | 102 | 25.922 | 26.313 | 38.237 | 1.00 | 47.07 | O |
| ATOM | 702 | N | TYR | A | 103 | 21.704 | 29.451 | 39.523 | 1.00 | 42.91 | N |
| ATOM | 703 | CA | TYR | A | 103 | 22.642 | 29.970 | 40.527 | 1.00 | 42.67 | C |
| ATOM | 704 | C | TYR | A | 103 | 23.561 | 28.895 | 41.102 | 1.00 | 41.98 | C |
| ATOM | 705 | O | TYR | A | 103 | 23.165 | 27.768 | 41.351 | 1.00 | 41.99 | O |
| ATOM | 706 | CB | TYR | A | 103 | 21.922 | 30.638 | 41.670 | 1.00 | 42.83 | C |
| ATOM | 707 | CG | TYR | A | 103 | 20.974 | 29.692 | 42.265 | 1.00 | 44.33 | C |
| ATOM | 708 | CD1 | TYR | A | 103 | 19.770 | 29.454 | 41.646 | 1.00 | 46.69 | C |
| ATOM | 709 | CD2 | TYR | A | 103 | 21.306 | 28.959 | 43.390 | 1.00 | 45.99 | C |
| ATOM | 710 | CE1 | TYR | A | 103 | 18.880 | 28.539 | 42.147 | 1.00 | 47.83 | C |
| ATOM | 711 | CE2 | TYR | A | 103 | 20.426 | 28.045 | 43.917 | 1.00 | 47.23 | C |
| ATOM | 712 | CZ | TYR | A | 103 | 19.203 | 27.836 | 43.284 | 1.00 | 48.65 | C |
| ATOM | 713 | OH | TYR | A | 103 | 18.287 | 26.921 | 43.774 | 1.00 | 51.36 | O |
| ATOM | 714 | N | ASP | A | 104 | 24.786 | 29.300 | 41.369 | 1.00 | 41.25 | N |
| ATOM | 715 | CA | ASP | A | 104 | 25.829 | 28.399 | 41.764 | 1.00 | 40.65 | C |
| ATOM | 716 | C | ASP | A | 104 | 25.924 | 28.335 | 43.267 | 1.00 | 40.45 | C |
| ATOM | 717 | O | ASP | A | 104 | 26.430 | 29.240 | 43.924 | 1.00 | 40.13 | O |
| ATOM | 718 | CB | ASP | A | 104 | 27.110 | 28.904 | 41.142 | 1.00 | 40.60 | C |
| ATOM | 719 | CG | ASP | A | 104 | 28.306 | 28.117 | 41.548 | 1.00 | 41.02 | C |
| ATOM | 720 | OD1 | ASP | A | 104 | 28.270 | 27.482 | 42.629 | 1.00 | 42.21 | O |
| ATOM | 721 | OD2 | ASP | A | 104 | 29.337 | 28.095 | 40.838 | 1.00 | 40.68 | O |
| ATOM | 722 | N | GLU | A | 105 | 25.446 | 27.222 | 43.801 | 1.00 | 40.41 | N |
| ATOM | 723 | CA | GLU | A | 105 | 25.368 | 27.029 | 45.231 | 1.00 | 40.21 | C |
| ATOM | 724 | C | GLU | A | 105 | 26.734 | 27.234 | 45.895 | 1.00 | 39.89 | C |
| ATOM | 725 | O | GLU | A | 105 | 26.803 | 27.738 | 47.021 | 1.00 | 39.65 | O |
| ATOM | 726 | CB | GLU | A | 105 | 24.769 | 25.643 | 45.528 | 1.00 | 40.44 | C |
| ATOM | 727 | CG | GLU | A | 105 | 23.247 | 25.572 | 45.351 | 1.00 | 41.43 | C |
| ATOM | 728 | CD | GLU | A | 105 | 22.708 | 24.150 | 45.207 | 1.00 | 42.48 | C |
| ATOM | 729 | OE1 | GLU | A | 105 | 23.138 | 23.269 | 45.986 | 1.00 | 43.10 | O |
| ATOM | 730 | OE2 | GLU | A | 105 | 21.842 | 23.914 | 44.322 | 1.00 | 42.00 | O |
| ATOM | 731 | N | LYS | A | 106 | 27.824 | 26.899 | 45.204 | 1.00 | 39.58 | N |
| ATOM | 732 | CA | LYS | A | 106 | 29.141 | 27.042 | 45.831 | 1.00 | 39.58 | C |
| ATOM | 733 | C | LYS | A | 106 | 29.427 | 28.469 | 46.190 | 1.00 | 39.64 | C |
| ATOM | 734 | O | LYS | A | 106 | 30.165 | 28.730 | 47.128 | 1.00 | 39.93 | O |
| ATOM | 735 | CB | LYS | A | 106 | 30.302 | 26.592 | 44.945 | 1.00 | 39.49 | C |
| ATOM | 736 | CG | LYS | A | 106 | 30.444 | 25.096 | 44.731 | 1.00 | 39.29 | C |
| ATOM | 737 | N | LYS | A | 107 | 28.856 | 29.397 | 45.438 | 1.00 | 39.68 | N |
| ATOM | 738 | CA | LYS | A | 107 | 29.140 | 30.794 | 45.663 | 1.00 | 39.58 | C |
| ATOM | 739 | C | LYS | A | 107 | 28.151 | 31.452 | 46.607 | 1.00 | 40.18 | C |
| ATOM | 740 | O | LYS | A | 107 | 28.279 | 32.637 | 46.883 | 1.00 | 40.30 | O |
| ATOM | 741 | CB | LYS | A | 107 | 29.161 | 31.531 | 44.325 | 1.00 | 39.46 | C |
| ATOM | 742 | CG | LYS | A | 107 | 30.390 | 31.199 | 43.455 | 1.00 | 38.46 | C |

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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 743 | CD | LYS A 107 | 30.299 | 31.737 | 42.029 | 1.00 | 36.98 | C |
| ATOM | 744 | CE | LYS A 107 | 31.643 | 31.632 | 41.292 | 1.00 | 36.36 | C |
| ATOM | 745 | NZ | LYS A 107 | 31.553 | 31.935 | 39.819 | 1.00 | 35.12 | N |
| ATOM | 746 | N | MET A 108 | 27.197 | 30.697 | 47.148 | 1.00 | 40.92 | N |
| ATOM | 747 | CA | MET A 108 | 26.165 | 31.316 | 47.978 | 1.00 | 41.42 | C |
| ATOM | 748 | C | MET A 108 | 26.675 | 31.937 | 49.258 | 1.00 | 42.03 | C |
| ATOM | 749 | O | MET A 108 | 26.142 | 32.952 | 49.704 | 1.00 | 42.33 | O |
| ATOM | 750 | CB | MET A 108 | 25.006 | 30.366 | 48.210 | 1.00 | 41.31 | C |
| ATOM | 751 | CG | MET A 108 | 24.285 | 30.179 | 46.892 | 1.00 | 41.95 | C |
| ATOM | 752 | SD | MET A 108 | 22.861 | 29.100 | 46.846 | 1.00 | 43.29 | S |
| ATOM | 753 | CE | MET A 108 | 21.737 | 30.010 | 48.064 | 1.00 | 43.04 | C |
| ATOM | 754 | N | ALA A 109 | 27.737 | 31.382 | 49.816 | 1.00 | 42.84 | N |
| ATOM | 755 | CA | ALA A 109 | 28.282 | 31.912 | 51.064 | 1.00 | 43.65 | C |
| ATOM | 756 | C | ALA A 109 | 28.655 | 33.387 | 50.963 | 1.00 | 44.40 | C |
| ATOM | 757 | O | ALA A 109 | 28.321 | 34.195 | 51.823 | 1.00 | 44.44 | O |
| ATOM | 758 | CB | ALA A 109 | 29.486 | 31.107 | 51.476 | 1.00 | 43.66 | C |
| ATOM | 759 | N | ASN A 110 | 29.332 | 33.729 | 49.882 | 1.00 | 45.46 | N |
| ATOM | 760 | CA | ASN A 110 | 29.817 | 35.084 | 49.665 | 1.00 | 46.25 | C |
| ATOM | 761 | C | ASN A 110 | 28.789 | 36.154 | 49.317 | 1.00 | 46.26 | C |
| ATOM | 762 | O | ASN A 110 | 29.163 | 37.304 | 49.066 | 1.00 | 46.51 | O |
| ATOM | 763 | CB | ASN A 110 | 30.841 | 35.036 | 48.543 | 1.00 | 46.62 | C |
| ATOM | 764 | CG | ASN A 110 | 32.024 | 34.145 | 48.886 | 1.00 | 47.94 | C |
| ATOM | 765 | OD1 | ASN A 110 | 32.474 | 34.093 | 50.045 | 1.00 | 48.12 | O |
| ATOM | 766 | ND2 | ASN A 110 | 32.530 | 33.432 | 47.883 | 1.00 | 48.75 | N |
| ATOM | 767 | N | PHE A 111 | 27.517 | 35.786 | 49.228 | 1.00 | 46.12 | N |
| ATOM | 768 | CA | PHE A 111 | 26.470 | 36.795 | 49.057 | 1.00 | 45.97 | C |
| ATOM | 769 | C | PHE A 111 | 25.267 | 36.385 | 49.889 | 1.00 | 46.17 | C |
| ATOM | 770 | O | PHE A 111 | 24.217 | 36.002 | 49.361 | 1.00 | 46.25 | O |
| ATOM | 771 | CB | PHE A 111 | 26.072 | 36.978 | 47.599 | 1.00 | 45.55 | C |
| ATOM | 772 | CG | PHE A 111 | 27.076 | 37.718 | 46.777 | 1.00 | 44.32 | C |
| ATOM | 773 | CD1 | PHE A 111 | 28.269 | 37.123 | 46.419 | 1.00 | 43.65 | C |
| ATOM | 774 | CD2 | PHE A 111 | 26.808 | 39.000 | 46.320 | 1.00 | 44.04 | C |
| ATOM | 775 | CE1 | PHE A 111 | 29.187 | 37.794 | 45.620 | 1.00 | 43.19 | C |
| ATOM | 776 | CE2 | PHE A 111 | 27.715 | 39.673 | 45.522 | 1.00 | 43.22 | C |
| ATOM | 777 | CZ | PHE A 111 | 28.911 | 39.068 | 45.177 | 1.00 | 43.00 | C |
| ATOM | 778 | N | GLN A 112 | 25.434 | 36.479 | 51.200 | 1.00 | 46.35 | N |
| ATOM | 779 | CA | GLN A 112 | 24.401 | 36.052 | 52.130 | 1.00 | 46.52 | C |
| ATOM | 780 | C | GLN A 112 | 23.040 | 36.638 | 51.754 | 1.00 | 46.68 | C |
| ATOM | 781 | O | GLN A 112 | 22.019 | 35.995 | 51.968 | 1.00 | 46.87 | O |
| ATOM | 782 | CB | GLN A 112 | 24.774 | 36.438 | 53.567 | 1.00 | 46.62 | C |
| ATOM | 783 | CG | GLN A 112 | 26.201 | 36.060 | 53.998 | 1.00 | 46.96 | C |
| ATOM | 784 | CD | GLN A 112 | 26.418 | 34.554 | 54.125 | 1.00 | 48.05 | C |
| ATOM | 785 | OE1 | GLN A 112 | 25.834 | 33.762 | 53.372 | 1.00 | 47.89 | O |
| ATOM | 786 | NE2 | GLN A 112 | 27.271 | 34.158 | 55.075 | 1.00 | 48.55 | N |
| ATOM | 787 | N | ASN A 113 | 23.019 | 37.836 | 51.168 | 1.00 | 46.80 | N |
| ATOM | 788 | CA | ASN A 113 | 21.750 | 38.463 | 50.793 | 1.00 | 46.89 | C |
| ATOM | 789 | C | ASN A 113 | 21.104 | 37.951 | 49.517 | 1.00 | 47.08 | C |
| ATOM | 790 | O | ASN A 113 | 20.105 | 38.521 | 49.077 | 1.00 | 47.55 | O |
| ATOM | 791 | CB | ASN A 113 | 21.898 | 39.976 | 50.682 | 1.00 | 46.69 | C |
| ATOM | 792 | CG | ASN A 113 | 22.258 | 40.604 | 52.001 | 1.00 | 46.91 | C |
| ATOM | 793 | OD1 | ASN A 113 | 22.085 | 39.982 | 53.055 | 1.00 | 46.08 | O |
| ATOM | 794 | ND2 | ASN A 113 | 22.767 | 41.837 | 51.962 | 1.00 | 46.59 | N |
| ATOM | 795 | N | PHE A 114 | 21.651 | 36.908 | 48.903 | 1.00 | 47.08 | N |
| ATOM | 796 | CA | PHE A 114 | 21.012 | 36.379 | 47.706 | 1.00 | 47.01 | C |
| ATOM | 797 | C | PHE A 114 | 19.986 | 35.364 | 48.145 | 1.00 | 47.11 | C |
| ATOM | 798 | O | PHE A 114 | 20.293 | 34.449 | 48.916 | 1.00 | 47.34 | O |
| ATOM | 799 | CB | PHE A 114 | 21.995 | 35.713 | 46.764 | 1.00 | 46.83 | C |
| ATOM | 800 | CG | PHE A 114 | 21.342 | 35.132 | 45.555 | 1.00 | 47.03 | C |
| ATOM | 801 | CD1 | PHE A 114 | 20.674 | 35.953 | 44.655 | 1.00 | 47.22 | C |
| ATOM | 802 | CD2 | PHE A 114 | 21.376 | 33.761 | 45.318 | 1.00 | 47.97 | C |
| ATOM | 803 | CE1 | PHE A 114 | 20.060 | 35.422 | 43.522 | 1.00 | 47.53 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 804 | CE2 | PHE | A | 114 | 20.763 | 33.212 | 44.177 | 1.00 | 47.83 | C |
| ATOM | 805 | CZ | PHE | A | 114 | 20.104 | 34.044 | 43.282 | 1.00 | 47.67 | C |
| ATOM | 806 | N | LYS | A | 115 | 18.763 | 35.530 | 47.662 | 1.00 | 46.94 | N |
| ATOM | 807 | CA | LYS | A | 115 | 17.683 | 34.628 | 48.029 | 1.00 | 46.64 | C |
| ATOM | 808 | C | LYS | A | 115 | 17.109 | 34.063 | 46.744 | 1.00 | 46.38 | C |
| ATOM | 809 | O | LYS | A | 115 | 16.351 | 34.744 | 46.046 | 1.00 | 46.75 | O |
| ATOM | 810 | CB | LYS | A | 115 | 16.613 | 35.372 | 48.835 | 1.00 | 46.60 | C |
| ATOM | 811 | N | PRO | A | 116 | 17.445 | 32.813 | 46.449 | 1.00 | 45.84 | N |
| ATOM | 812 | CA | PRO | A | 116 | 17.079 | 32.192 | 45.165 | 1.00 | 45.70 | C |
| ATOM | 813 | C | PRO | A | 116 | 15.576 | 32.139 | 44.937 | 1.00 | 45.44 | C |
| ATOM | 814 | O | PRO | A | 116 | 14.827 | 31.956 | 45.892 | 1.00 | 45.46 | O |
| ATOM | 815 | CB | PRO | A | 116 | 17.640 | 30.761 | 45.260 | 1.00 | 45.71 | C |
| ATOM | 816 | CG | PRO | A | 116 | 18.435 | 30.689 | 46.536 | 1.00 | 45.66 | C |
| ATOM | 817 | CD | PRO | A | 116 | 18.137 | 31.890 | 47.359 | 1.00 | 45.75 | C |
| ATOM | 818 | N | ARG | A | 117 | 15.154 | 32.307 | 43.688 | 1.00 | 45.27 | N |
| ATOM | 819 | CA | ARG | A | 117 | 13.742 | 32.232 | 43.332 | 1.00 | 45.16 | C |
| ATOM | 820 | C | ARG | A | 117 | 13.291 | 30.791 | 43.104 | 1.00 | 45.12 | C |
| ATOM | 821 | O | ARG | A | 117 | 12.096 | 30.500 | 43.207 | 1.00 | 45.48 | O |
| ATOM | 822 | CB | ARG | A | 117 | 13.467 | 33.059 | 42.097 | 1.00 | 45.26 | C |
| ATOM | 823 | N | SER | A | 118 | 14.238 | 29.902 | 42.796 | 1.00 | 44.78 | N |
| ATOM | 824 | CA | SER | A | 118 | 13.944 | 28.480 | 42.594 | 1.00 | 44.60 | C |
| ATOM | 825 | C | SER | A | 118 | 14.782 | 27.583 | 43.509 | 1.00 | 44.63 | C |
| ATOM | 826 | O | SER | A | 118 | 15.925 | 27.921 | 43.816 | 1.00 | 45.32 | O |
| ATOM | 827 | CB | SER | A | 118 | 14.303 | 28.072 | 41.184 | 1.00 | 44.44 | C |
| ATOM | 828 | OG | SER | A | 118 | 15.651 | 27.624 | 41.186 | 1.00 | 44.35 | O |
| ATOM | 829 | N | ASN | A | 119 | 14.241 | 26.428 | 43.899 | 1.00 | 44.11 | N |
| ATOM | 830 | CA | ASN | A | 119 | 14.969 | 25.472 | 44.728 | 1.00 | 43.72 | C |
| ATOM | 831 | C | ASN | A | 119 | 15.295 | 24.196 | 43.953 | 1.00 | 43.16 | C |
| ATOM | 832 | O | ASN | A | 119 | 14.576 | 23.821 | 43.030 | 1.00 | 43.23 | O |
| ATOM | 833 | CB | ASN | A | 119 | 14.147 | 25.078 | 45.955 | 1.00 | 44.03 | C |
| ATOM | 834 | CG | ASN | A | 119 | 13.514 | 26.264 | 46.646 | 1.00 | 44.80 | C |
| ATOM | 835 | OD1 | ASN | A | 119 | 14.207 | 27.129 | 47.197 | 1.00 | 46.56 | O |
| ATOM | 836 | ND2 | ASN | A | 119 | 12.184 | 26.303 | 46.640 | 1.00 | 45.18 | N |
| ATOM | 837 | N | ARG | A | 120 | 16.380 | 23.533 | 44.337 | 1.00 | 42.37 | N |
| ATOM | 838 | CA | ARG | A | 120 | 16.778 | 22.278 | 43.716 | 1.00 | 41.69 | C |
| ATOM | 839 | C | ARG | A | 120 | 16.368 | 21.162 | 44.656 | 1.00 | 41.20 | C |
| ATOM | 840 | O | ARG | A | 120 | 16.577 | 21.267 | 45.859 | 1.00 | 41.46 | O |
| ATOM | 841 | CB | ARG | A | 120 | 18.299 | 22.239 | 43.504 | 1.00 | 41.70 | C |
| ATOM | 842 | CG | ARG | A | 120 | 18.827 | 21.002 | 42.754 | 1.00 | 40.96 | C |
| ATOM | 843 | CD | ARG | A | 120 | 20.351 | 20.897 | 42.683 | 1.00 | 39.92 | C |
| ATOM | 844 | NE | ARG | A | 120 | 21.001 | 21.327 | 43.920 | 1.00 | 39.89 | N |
| ATOM | 845 | CZ | ARG | A | 120 | 21.337 | 20.523 | 44.921 | 1.00 | 39.57 | C |
| ATOM | 846 | NH1 | ARG | A | 120 | 21.084 | 19.217 | 44.856 | 1.00 | 39.43 | N |
| ATOM | 847 | NH2 | ARG | A | 120 | 21.930 | 21.027 | 45.998 | 1.00 | 39.06 | N |
| ATOM | 848 | N | GLU | A | 121 | 15.769 | 20.109 | 44.115 | 1.00 | 40.44 | N |
| ATOM | 849 | CA | GLU | A | 121 | 15.380 | 18.956 | 44.908 | 1.00 | 39.92 | C |
| ATOM | 850 | C | GLU | A | 121 | 15.840 | 17.702 | 44.161 | 1.00 | 39.36 | C |
| ATOM | 851 | O | GLU | A | 121 | 15.716 | 17.617 | 42.942 | 1.00 | 39.20 | O |
| ATOM | 852 | CB | GLU | A | 121 | 13.866 | 18.950 | 45.170 | 1.00 | 39.97 | C |
| ATOM | 853 | CG | GLU | A | 121 | 13.369 | 17.698 | 45.876 | 1.00 | 40.42 | C |
| ATOM | 854 | CD | GLU | A | 121 | 12.136 | 17.928 | 46.731 | 1.00 | 41.22 | C |
| ATOM | 855 | OE1 | GLU | A | 121 | 12.291 | 18.365 | 47.890 | 1.00 | 41.90 | O |
| ATOM | 856 | OE2 | GLU | A | 121 | 11.016 | 17.645 | 46.259 | 1.00 | 42.21 | O |
| ATOM | 857 | N | GLU | A | 122 | 16.414 | 16.752 | 44.889 | 1.00 | 38.78 | N |
| ATOM | 858 | CA | GLU | A | 122 | 16.879 | 15.519 | 44.285 | 1.00 | 38.34 | C |
| ATOM | 859 | C | GLU | A | 122 | 15.760 | 14.523 | 44.374 | 1.00 | 38.13 | C |
| ATOM | 860 | O | GLU | A | 122 | 15.171 | 14.353 | 45.435 | 1.00 | 38.09 | O |
| ATOM | 861 | CB | GLU | A | 122 | 18.092 | 14.989 | 45.025 | 1.00 | 38.08 | C |
| ATOM | 862 | CG | GLU | A | 122 | 19.263 | 15.928 | 44.936 | 1.00 | 38.04 | C |
| ATOM | 863 | CD | GLU | A | 122 | 19.581 | 16.289 | 43.497 | 1.00 | 39.25 | C |
| ATOM | 864 | OE1 | GLU | A | 122 | 19.763 | 15.364 | 42.667 | 1.00 | 38.89 | O |

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ATOM    865  OE2 GLU A 122      19.627  17.501  43.183  1.00 40.06           O
ATOM    866  N   MET A 123      15.434  13.879  43.265  1.00 37.93           N
ATOM    867  CA  MET A 123      14.384  12.885  43.312  1.00 37.84           C
ATOM    868  C   MET A 123      14.536  11.819  42.242  1.00 37.41           C
ATOM    869  O   MET A 123      15.418  11.876  41.387  1.00 37.04           O
ATOM    870  CB  MET A 123      13.021  13.565  43.225  1.00 38.01           C
ATOM    871  CG  MET A 123      12.798  14.318  41.946  1.00 39.05           C
ATOM    872  SD  MET A 123      11.177  15.064  41.910  1.00 41.38           S
ATOM    873  CE  MET A 123      11.489  16.589  42.818  1.00 41.39           C
ATOM    874  N   LYS A 124      13.675  10.820  42.332  1.00 37.17           N
ATOM    875  CA  LYS A 124      13.692   9.715  41.401  1.00 36.98           C
ATOM    876  C   LYS A 124      12.802  10.098  40.238  1.00 36.81           C
ATOM    877  O   LYS A 124      11.814  10.813  40.402  1.00 36.91           O
ATOM    878  CB  LYS A 124      13.213   8.434  42.087  1.00 36.82           C
ATOM    879  CG  LYS A 124      14.081   7.989  43.281  1.00 36.79           C
ATOM    880  CD  LYS A 124      15.488   7.553  42.856  1.00 36.83           C
ATOM    881  CE  LYS A 124      16.390   7.206  44.031  1.00 36.89           C
ATOM    882  NZ  LYS A 124      17.822   7.412  43.680  1.00 36.99           N
ATOM    883  N   PHE A 125      13.145   9.622  39.056  1.00 36.49           N
ATOM    884  CA  PHE A 125      12.416  10.031  37.885  1.00 36.33           C
ATOM    885  C   PHE A 125      10.926   9.861  38.074  1.00 36.45           C
ATOM    886  O   PHE A 125      10.143  10.743  37.732  1.00 36.30           O
ATOM    887  CB  PHE A 125      12.879   9.270  36.665  1.00 36.24           C
ATOM    888  CG  PHE A 125      12.555   9.967  35.407  1.00 36.21           C
ATOM    889  CD1 PHE A 125      13.403  10.936  34.924  1.00 35.98           C
ATOM    890  CD2 PHE A 125      11.374   9.714  34.743  1.00 36.15           C
ATOM    891  CE1 PHE A 125      13.108  11.616  33.794  1.00 36.07           C
ATOM    892  CE2 PHE A 125      11.073  10.390  33.597  1.00 36.71           C
ATOM    893  CZ  PHE A 125      11.943  11.350  33.120  1.00 36.73           C
ATOM    894  N   HIS A 126      10.527   8.733  38.640  1.00 36.80           N
ATOM    895  CA  HIS A 126       9.111   8.492  38.845  1.00 36.98           C
ATOM    896  C   HIS A 126       8.547   9.560  39.772  1.00 37.20           C
ATOM    897  O   HIS A 126       7.376   9.923  39.669  1.00 37.15           O
ATOM    898  CB  HIS A 126       8.845   7.080  39.390  1.00 36.97           C
ATOM    899  CG  HIS A 126       8.990   6.946  40.877  1.00 36.62           C
ATOM    900  ND1 HIS A 126       7.935   7.115  41.747  1.00 35.91           N
ATOM    901  CD2 HIS A 126      10.058   6.618  41.644  1.00 36.38           C
ATOM    902  CE1 HIS A 126       8.352   6.921  42.986  1.00 35.63           C
ATOM    903  NE2 HIS A 126       9.636   6.619  42.951  1.00 35.43           N
ATOM    904  N   GLU A 127       9.383  10.082  40.663  1.00 37.34           N
ATOM    905  CA  GLU A 127       8.912  11.087  41.599  1.00 37.55           C
ATOM    906  C   GLU A 127       8.657  12.379  40.835  1.00 37.54           C
ATOM    907  O   GLU A 127       7.657  13.061  41.049  1.00 37.36           O
ATOM    908  CB  GLU A 127       9.914  11.308  42.736  1.00 37.65           C
ATOM    909  CG  GLU A 127      10.155  10.091  43.617  1.00 37.89           C
ATOM    910  CD  GLU A 127      11.113  10.383  44.764  1.00 38.14           C
ATOM    911  OE1 GLU A 127      12.330  10.531  44.520  1.00 37.77           O
ATOM    912  OE2 GLU A 127      10.649  10.471  45.917  1.00 38.86           O
ATOM    913  N   PHE A 128       9.557  12.702  39.920  1.00 37.65           N
ATOM    914  CA  PHE A 128       9.393  13.904  39.127  1.00 37.81           C
ATOM    915  C   PHE A 128       8.090  13.798  38.350  1.00 37.95           C
ATOM    916  O   PHE A 128       7.280  14.726  38.342  1.00 37.90           O
ATOM    917  CB  PHE A 128      10.578  14.061  38.173  1.00 37.88           C
ATOM    918  CG  PHE A 128      10.332  15.012  37.028  1.00 37.52           C
ATOM    919  CD1 PHE A 128      10.088  16.355  37.258  1.00 36.94           C
ATOM    920  CD2 PHE A 128      10.380  14.559  35.720  1.00 37.02           C
ATOM    921  CE1 PHE A 128       9.876  17.219  36.203  1.00 37.09           C
ATOM    922  CE2 PHE A 128      10.170  15.423  34.663  1.00 37.21           C
ATOM    923  CZ  PHE A 128       9.917  16.748  34.901  1.00 37.15           C
ATOM    924  N   VAL A 129       7.878  12.646  37.726  1.00 38.00           N
ATOM    925  CA  VAL A 129       6.716  12.454  36.876  1.00 38.16           C
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ATOM    926  C   VAL A 129       5.442  12.637  37.671  1.00 38.24           C
ATOM    927  O   VAL A 129       4.494  13.286  37.224  1.00 38.04           O
ATOM    928  CB  VAL A 129       6.705  11.050  36.268  1.00 38.36           C
ATOM    929  CG1 VAL A 129       5.398  10.810  35.508  1.00 38.41           C
ATOM    930  CG2 VAL A 129       7.935  10.841  35.372  1.00 38.22           C
ATOM    931  N   GLU A 130       5.430  12.038  38.854  1.00 38.42           N
ATOM    932  CA  GLU A 130       4.289  12.115  39.745  1.00 38.54           C
ATOM    933  C   GLU A 130       4.025  13.578  40.083  1.00 38.43           C
ATOM    934  O   GLU A 130       2.898  14.056  39.960  1.00 38.29           O
ATOM    935  CB  GLU A 130       4.547  11.265  40.997  1.00 38.69           C
ATOM    936  CG  GLU A 130       4.404   9.763  40.745  1.00 39.15           C
ATOM    937  CD  GLU A 130       5.160   8.897  41.740  1.00 39.75           C
ATOM    938  OE1 GLU A 130       5.551   9.403  42.815  1.00 40.08           O
ATOM    939  OE2 GLU A 130       5.355   7.697  41.441  1.00 40.15           O
ATOM    940  N   LYS A 131       5.070  14.299  40.471  1.00 38.39           N
ATOM    941  CA  LYS A 131       4.908  15.707  40.787  1.00 38.52           C
ATOM    942  C   LYS A 131       4.290  16.431  39.598  1.00 38.61           C
ATOM    943  O   LYS A 131       3.393  17.252  39.769  1.00 38.51           O
ATOM    944  CB  LYS A 131       6.240  16.356  41.149  1.00 38.58           C
ATOM    945  CG  LYS A 131       6.440  16.666  42.625  1.00 38.76           C
ATOM    946  CD  LYS A 131       7.045  18.060  42.753  1.00 39.73           C
ATOM    947  CE  LYS A 131       7.756  18.316  44.070  1.00 40.49           C
ATOM    948  NZ  LYS A 131       8.117  19.772  44.197  1.00 40.68           N
ATOM    949  N   LEU A 132       4.764  16.136  38.391  1.00 38.84           N
ATOM    950  CA  LEU A 132       4.196  16.771  37.208  1.00 39.00           C
ATOM    951  C   LEU A 132       2.726  16.429  37.113  1.00 39.11           C
ATOM    952  O   LEU A 132       1.903  17.287  36.810  1.00 39.20           O
ATOM    953  CB  LEU A 132       4.894  16.328  35.932  1.00 38.96           C
ATOM    954  CG  LEU A 132       6.287  16.899  35.723  1.00 39.44           C
ATOM    955  CD1 LEU A 132       6.870  16.389  34.429  1.00 39.81           C
ATOM    956  CD2 LEU A 132       6.261  18.421  35.709  1.00 40.07           C
ATOM    957  N   GLN A 133       2.396  15.170  37.367  1.00 39.22           N
ATOM    958  CA  GLN A 133       1.005  14.758  37.335  1.00 39.38           C
ATOM    959  C   GLN A 133       0.172  15.523  38.370  1.00 39.57           C
ATOM    960  O   GLN A 133      -0.893  16.034  38.029  1.00 39.48           O
ATOM    961  CB  GLN A 133       0.874  13.250  37.536  1.00 39.22           C
ATOM    962  N   ASP A 134       0.656  15.631  39.611  1.00 39.91           N
ATOM    963  CA  ASP A 134      -0.129  16.279  40.677  1.00 40.29           C
ATOM    964  C   ASP A 134      -0.437  17.732  40.379  1.00 40.17           C
ATOM    965  O   ASP A 134      -1.543  18.211  40.623  1.00 40.02           O
ATOM    966  CB  ASP A 134       0.564  16.198  42.041  1.00 40.57           C
ATOM    967  CG  ASP A 134      -0.348  16.660  43.182  1.00 41.99           C
ATOM    968  OD1 ASP A 134      -1.301  17.421  42.910  1.00 43.76           O
ATOM    969  OD2 ASP A 134      -0.212  16.312  44.378  1.00 44.05           O
ATOM    970  N   ILE A 135       0.545  18.438  39.846  1.00 40.17           N
ATOM    971  CA  ILE A 135       0.350  19.836  39.556  1.00 40.10           C
ATOM    972  C   ILE A 135      -0.719  19.973  38.500  1.00 40.10           C
ATOM    973  O   ILE A 135      -1.648  20.759  38.652  1.00 40.26           O
ATOM    974  CB  ILE A 135       1.639  20.455  39.085  1.00 40.10           C
ATOM    975  CG1 ILE A 135       2.612  20.560  40.261  1.00 40.11           C
ATOM    976  CG2 ILE A 135       1.358  21.817  38.507  1.00 40.22           C
ATOM    977  CD1 ILE A 135       4.056  20.688  39.842  1.00 40.17           C
ATOM    978  N   GLN A 136      -0.596  19.198  37.431  1.00 40.02           N
ATOM    979  CA  GLN A 136      -1.586  19.248  36.376  1.00 39.96           C
ATOM    980  C   GLN A 136      -2.956  19.094  37.000  1.00 39.99           C
ATOM    981  O   GLN A 136      -3.795  19.991  36.921  1.00 39.86           O
ATOM    982  CB  GLN A 136      -1.350  18.144  35.361  1.00 40.00           C
ATOM    983  N   GLN A 137      -3.158  17.972  37.679  1.00 40.18           N
ATOM    984  CA  GLN A 137      -4.486  17.630  38.164  1.00 40.31           C
ATOM    985  C   GLN A 137      -4.995  18.683  39.114  1.00 40.45           C
ATOM    986  O   GLN A 137      -6.170  19.046  39.068  1.00 40.75           O
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 987 | CB | GLN | A | 137 | -4.502 | 16.247 | 38.829 | 1.00 | 40.24 | C |
| ATOM | 988 | N | ARG | A | 138 | -4.116 | 19.200 | 39.959 | 1.00 | 40.45 | N |
| ATOM | 989 | CA | ARG | A | 138 | -4.560 | 20.159 | 40.956 | 1.00 | 40.45 | C |
| ATOM | 990 | C | ARG | A | 138 | -4.568 | 21.588 | 40.419 | 1.00 | 40.54 | C |
| ATOM | 991 | O | ARG | A | 138 | -4.678 | 22.541 | 41.188 | 1.00 | 40.67 | O |
| ATOM | 992 | CB | ARG | A | 138 | -3.692 | 20.069 | 42.207 | 1.00 | 40.43 | C |
| ATOM | 993 | CG | ARG | A | 138 | -2.399 | 20.868 | 42.161 | 1.00 | 40.03 | C |
| ATOM | 994 | CD | ARG | A | 138 | -1.541 | 20.546 | 43.346 | 1.00 | 39.94 | C |
| ATOM | 995 | NE | ARG | A | 138 | -0.431 | 21.458 | 43.580 | 1.00 | 39.71 | N |
| ATOM | 996 | CZ | ARG | A | 138 | 0.842 | 21.098 | 43.498 | 1.00 | 40.13 | C |
| ATOM | 997 | NH1 | ARG | A | 138 | 1.164 | 19.857 | 43.150 | 1.00 | 40.53 | N |
| ATOM | 998 | NH2 | ARG | A | 138 | 1.800 | 21.978 | 43.747 | 1.00 | 40.33 | N |
| ATOM | 999 | N | GLY | A | 139 | -4.471 | 21.742 | 39.102 | 1.00 | 40.47 | N |
| ATOM | 1000 | CA | GLY | A | 139 | -4.418 | 23.066 | 38.508 | 1.00 | 40.46 | C |
| ATOM | 1001 | C | GLY | A | 139 | -3.432 | 24.021 | 39.176 | 1.00 | 40.45 | C |
| ATOM | 1002 | O | GLY | A | 139 | -3.616 | 25.235 | 39.110 | 1.00 | 40.46 | O |
| ATOM | 1003 | N | GLY | A | 140 | -2.370 | 23.490 | 39.780 | 1.00 | 40.47 | N |
| ATOM | 1004 | CA | GLY | A | 140 | -1.425 | 24.314 | 40.519 | 1.00 | 40.45 | C |
| ATOM | 1005 | C | GLY | A | 140 | -0.695 | 25.272 | 39.602 | 1.00 | 40.40 | C |
| ATOM | 1006 | O | GLY | A | 140 | -0.784 | 25.116 | 38.383 | 1.00 | 40.79 | O |
| ATOM | 1007 | N | GLU | A | 141 | -0.015 | 26.273 | 40.167 | 1.00 | 40.10 | N |
| ATOM | 1008 | CA | GLU | A | 141 | 0.807 | 27.195 | 39.371 | 1.00 | 40.01 | C |
| ATOM | 1009 | C | GLU | A | 141 | 2.305 | 26.854 | 39.458 | 1.00 | 39.64 | C |
| ATOM | 1010 | O | GLU | A | 141 | 3.112 | 27.386 | 38.692 | 1.00 | 39.52 | O |
| ATOM | 1011 | CB | GLU | A | 141 | 0.589 | 28.660 | 39.796 | 1.00 | 40.20 | C |
| ATOM | 1012 | CG | GLU | A | 141 | -0.711 | 29.298 | 39.315 | 1.00 | 41.00 | C |
| ATOM | 1013 | CD | GLU | A | 141 | -0.845 | 29.307 | 37.800 | 1.00 | 42.10 | C |
| ATOM | 1014 | OE1 | GLU | A | 141 | 0.194 | 29.181 | 37.113 | 1.00 | 41.99 | O |
| ATOM | 1015 | OE2 | GLU | A | 141 | -1.990 | 29.437 | 37.300 | 1.00 | 43.15 | O |
| ATOM | 1016 | N | GLU | A | 142 | 2.676 | 25.977 | 40.392 | 1.00 | 39.25 | N |
| ATOM | 1017 | CA | GLU | A | 142 | 4.075 | 25.589 | 40.563 | 1.00 | 38.95 | C |
| ATOM | 1018 | C | GLU | A | 142 | 4.613 | 25.162 | 39.210 | 1.00 | 38.74 | C |
| ATOM | 1019 | O | GLU | A | 142 | 3.859 | 24.694 | 38.351 | 1.00 | 38.77 | O |
| ATOM | 1020 | CB | GLU | A | 142 | 4.220 | 24.433 | 41.577 | 1.00 | 38.95 | C |
| ATOM | 1021 | CG | GLU | A | 142 | 5.658 | 24.138 | 42.019 | 1.00 | 38.90 | C |
| ATOM | 1022 | CD | GLU | A | 142 | 5.797 | 22.950 | 42.971 | 1.00 | 38.93 | C |
| ATOM | 1023 | OE1 | GLU | A | 142 | 4.836 | 22.164 | 43.130 | 1.00 | 39.58 | O |
| ATOM | 1024 | OE2 | GLU | A | 142 | 6.888 | 22.799 | 43.565 | 1.00 | 38.74 | O |
| ATOM | 1025 | N | ARG | A | 143 | 5.914 | 25.332 | 39.020 | 1.00 | 38.39 | N |
| ATOM | 1026 | CA | ARG | A | 143 | 6.569 | 24.908 | 37.796 | 1.00 | 38.25 | C |
| ATOM | 1027 | C | ARG | A | 143 | 7.809 | 24.122 | 38.122 | 1.00 | 38.14 | C |
| ATOM | 1028 | O | ARG | A | 143 | 8.512 | 24.450 | 39.078 | 1.00 | 38.46 | O |
| ATOM | 1029 | CB | ARG | A | 143 | 7.046 | 26.107 | 37.003 | 1.00 | 38.26 | C |
| ATOM | 1030 | CG | ARG | A | 143 | 5.986 | 26.945 | 36.398 | 1.00 | 37.89 | C |
| ATOM | 1031 | CD | ARG | A | 143 | 6.602 | 28.026 | 35.555 | 1.00 | 37.35 | C |
| ATOM | 1032 | NE | ARG | A | 143 | 5.610 | 28.814 | 34.849 | 1.00 | 36.66 | N |
| ATOM | 1033 | CZ | ARG | A | 143 | 5.316 | 28.668 | 33.573 | 1.00 | 36.40 | C |
| ATOM | 1034 | NH1 | ARG | A | 143 | 5.933 | 27.755 | 32.831 | 1.00 | 36.41 | N |
| ATOM | 1035 | NH2 | ARG | A | 143 | 4.397 | 29.443 | 33.034 | 1.00 | 37.02 | N |
| ATOM | 1036 | N | LEU | A | 144 | 8.116 | 23.124 | 37.304 | 1.00 | 37.71 | N |
| ATOM | 1037 | CA | LEU | A | 144 | 9.319 | 22.349 | 37.517 | 1.00 | 37.57 | C |
| ATOM | 1038 | C | LEU | A | 144 | 10.181 | 22.319 | 36.294 | 1.00 | 37.33 | C |
| ATOM | 1039 | O | LEU | A | 144 | 9.710 | 22.466 | 35.165 | 1.00 | 37.31 | O |
| ATOM | 1040 | CB | LEU | A | 144 | 8.979 | 20.909 | 37.858 | 1.00 | 37.69 | C |
| ATOM | 1041 | CG | LEU | A | 144 | 7.981 | 20.736 | 38.993 | 1.00 | 38.31 | C |
| ATOM | 1042 | CD1 | LEU | A | 144 | 7.612 | 19.255 | 39.165 | 1.00 | 39.02 | C |
| ATOM | 1043 | CD2 | LEU | A | 144 | 8.551 | 21.327 | 40.263 | 1.00 | 37.91 | C |
| ATOM | 1044 | N | TYR | A | 145 | 11.460 | 22.098 | 36.528 | 1.00 | 37.01 | N |
| ATOM | 1045 | CA | TYR | A | 145 | 12.379 | 21.922 | 35.437 | 1.00 | 36.87 | C |
| ATOM | 1046 | C | TYR | A | 145 | 13.397 | 20.886 | 35.871 | 1.00 | 36.85 | C |
| ATOM | 1047 | O | TYR | A | 145 | 14.146 | 21.093 | 36.819 | 1.00 | 36.51 | O |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1048 | CB | TYR | A | 145 | 13.043 | 23.255 | 35.110 | 1.00 | 36.92 | C |
| ATOM | 1049 | CG | TYR | A | 145 | 13.505 | 23.446 | 33.686 | 1.00 | 36.38 | C |
| ATOM | 1050 | CD1 | TYR | A | 145 | 13.845 | 22.383 | 32.875 | 1.00 | 36.31 | C |
| ATOM | 1051 | CD2 | TYR | A | 145 | 13.619 | 24.716 | 33.163 | 1.00 | 36.28 | C |
| ATOM | 1052 | CE1 | TYR | A | 145 | 14.278 | 22.590 | 31.582 | 1.00 | 36.21 | C |
| ATOM | 1053 | CE2 | TYR | A | 145 | 14.047 | 24.923 | 31.880 | 1.00 | 35.94 | C |
| ATOM | 1054 | CZ | TYR | A | 145 | 14.374 | 23.862 | 31.093 | 1.00 | 35.54 | C |
| ATOM | 1055 | OH | TYR | A | 145 | 14.789 | 24.081 | 29.799 | 1.00 | 36.13 | O |
| ATOM | 1056 | N | LEU | A | 146 | 13.378 | 19.736 | 35.218 | 1.00 | 37.06 | N |
| ATOM | 1057 | CA | LEU | A | 146 | 14.396 | 18.742 | 35.477 | 1.00 | 37.49 | C |
| ATOM | 1058 | C | LEU | A | 146 | 15.628 | 19.029 | 34.629 | 1.00 | 37.55 | C |
| ATOM | 1059 | O | LEU | A | 146 | 15.532 | 19.241 | 33.427 | 1.00 | 37.31 | O |
| ATOM | 1060 | CB | LEU | A | 146 | 13.877 | 17.341 | 35.173 | 1.00 | 37.69 | C |
| ATOM | 1061 | CG | LEU | A | 146 | 14.919 | 16.233 | 35.349 | 1.00 | 37.95 | C |
| ATOM | 1062 | CD1 | LEU | A | 146 | 14.234 | 14.916 | 35.567 | 1.00 | 37.66 | C |
| ATOM | 1063 | CD2 | LEU | A | 146 | 15.849 | 16.133 | 34.151 | 1.00 | 39.00 | C |
| ATOM | 1064 | N | GLN | A | 147 | 16.786 | 18.993 | 35.269 | 1.00 | 37.84 | N |
| ATOM | 1065 | CA | GLN | A | 147 | 18.053 | 19.259 | 34.617 | 1.00 | 38.09 | C |
| ATOM | 1066 | C | GLN | A | 147 | 19.088 | 18.397 | 35.306 | 1.00 | 37.92 | C |
| ATOM | 1067 | O | GLN | A | 147 | 19.453 | 18.661 | 36.443 | 1.00 | 37.87 | O |
| ATOM | 1068 | CB | GLN | A | 147 | 18.421 | 20.725 | 34.773 | 1.00 | 38.37 | C |
| ATOM | 1069 | CG | GLN | A | 147 | 17.331 | 21.686 | 34.362 | 1.00 | 39.01 | C |
| ATOM | 1070 | CD | GLN | A | 147 | 17.867 | 23.064 | 34.191 | 1.00 | 39.92 | C |
| ATOM | 1071 | OE1 | GLN | A | 147 | 17.149 | 23.955 | 33.772 | 1.00 | 42.51 | O |
| ATOM | 1072 | NE2 | GLN | A | 147 | 19.137 | 23.253 | 34.520 | 1.00 | 40.24 | N |
| ATOM | 1073 | N | GLN | A | 148 | 19.576 | 17.385 | 34.601 | 1.00 | 37.81 | N |
| ATOM | 1074 | CA | GLN | A | 148 | 20.433 | 16.377 | 35.196 | 1.00 | 37.57 | C |
| ATOM | 1075 | C | GLN | A | 148 | 21.325 | 15.744 | 34.176 | 1.00 | 37.68 | C |
| ATOM | 1076 | O | GLN | A | 148 | 20.876 | 15.266 | 33.146 | 1.00 | 37.30 | O |
| ATOM | 1077 | CB | GLN | A | 148 | 19.576 | 15.261 | 35.773 | 1.00 | 37.61 | C |
| ATOM | 1078 | CG | GLN | A | 148 | 20.336 | 13.971 | 36.068 | 1.00 | 36.79 | C |
| ATOM | 1079 | CD | GLN | A | 148 | 21.398 | 14.159 | 37.117 | 1.00 | 35.97 | C |
| ATOM | 1080 | OE1 | GLN | A | 148 | 21.162 | 14.814 | 38.135 | 1.00 | 35.11 | O |
| ATOM | 1081 | NE2 | GLN | A | 148 | 22.577 | 13.593 | 36.875 | 1.00 | 35.03 | N |
| ATOM | 1082 | N | THR | A | 149 | 22.596 | 15.698 | 34.503 | 1.00 | 38.15 | N |
| ATOM | 1083 | CA | THR | A | 149 | 23.574 | 15.130 | 33.622 | 1.00 | 38.57 | C |
| ATOM | 1084 | C | THR | A | 149 | 23.354 | 13.647 | 33.506 | 1.00 | 38.68 | C |
| ATOM | 1085 | O | THR | A | 149 | 23.154 | 12.973 | 34.509 | 1.00 | 39.07 | O |
| ATOM | 1086 | CB | THR | A | 149 | 24.936 | 15.410 | 34.214 | 1.00 | 38.75 | C |
| ATOM | 1087 | OG1 | THR | A | 149 | 25.206 | 16.807 | 34.088 | 1.00 | 38.86 | O |
| ATOM | 1088 | CG2 | THR | A | 149 | 26.036 | 14.759 | 33.418 | 1.00 | 39.39 | C |
| ATOM | 1089 | N | LEU | A | 150 | 23.393 | 13.144 | 32.279 | 1.00 | 38.87 | N |
| ATOM | 1090 | CA | LEU | A | 150 | 23.259 | 11.722 | 32.021 | 1.00 | 39.24 | C |
| ATOM | 1091 | C | LEU | A | 150 | 24.498 | 10.979 | 32.507 | 1.00 | 39.20 | C |
| ATOM | 1092 | O | LEU | A | 150 | 25.602 | 11.317 | 32.101 | 1.00 | 39.20 | O |
| ATOM | 1093 | CB | LEU | A | 150 | 23.146 | 11.465 | 30.519 | 1.00 | 39.46 | C |
| ATOM | 1094 | CG | LEU | A | 150 | 21.938 | 11.942 | 29.722 | 1.00 | 40.52 | C |
| ATOM | 1095 | CD1 | LEU | A | 150 | 22.077 | 11.563 | 28.237 | 1.00 | 41.06 | C |
| ATOM | 1096 | CD2 | LEU | A | 150 | 20.712 | 11.308 | 30.303 | 1.00 | 41.66 | C |
| ATOM | 1097 | N | ASN | A | 151 | 24.315 | 9.960 | 33.343 | 1.00 | 39.19 | N |
| ATOM | 1098 | CA | ASN | A | 151 | 25.436 | 9.171 | 33.861 | 1.00 | 39.46 | C |
| ATOM | 1099 | C | ASN | A | 151 | 25.193 | 7.642 | 33.883 | 1.00 | 39.43 | C |
| ATOM | 1100 | O | ASN | A | 151 | 24.198 | 7.162 | 33.333 | 1.00 | 39.15 | O |
| ATOM | 1101 | CB | ASN | A | 151 | 25.731 | 9.652 | 35.265 | 1.00 | 39.54 | C |
| ATOM | 1102 | CG | ASN | A | 151 | 24.511 | 9.588 | 36.150 | 1.00 | 40.08 | C |
| ATOM | 1103 | OD1 | ASN | A | 151 | 23.874 | 8.533 | 36.283 | 1.00 | 39.68 | O |
| ATOM | 1104 | ND2 | ASN | A | 151 | 24.158 | 10.725 | 36.751 | 1.00 | 40.83 | N |
| ATOM | 1105 | N | ASP | A | 152 | 26.075 | 6.892 | 34.556 | 1.00 | 39.43 | N |
| ATOM | 1106 | CA | ASP | A | 152 | 26.025 | 5.413 | 34.543 | 1.00 | 39.58 | C |
| ATOM | 1107 | C | ASP | A | 152 | 24.761 | 4.787 | 35.083 | 1.00 | 39.17 | C |
| ATOM | 1108 | O | ASP | A | 152 | 24.477 | 3.634 | 34.776 | 1.00 | 39.29 | O |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1109 | CB | ASP | A | 152 | 27.138 | 4.756 | 35.385 | 1.00 | 39.92 | C |
| ATOM | 1110 | CG | ASP | A | 152 | 28.489 | 5.382 | 35.198 | 1.00 | 41.53 | C |
| ATOM | 1111 | OD1 | ASP | A | 152 | 28.722 | 6.005 | 34.134 | 1.00 | 45.10 | O |
| ATOM | 1112 | OD2 | ASP | A | 152 | 29.378 | 5.294 | 36.076 | 1.00 | 42.02 | O |
| ATOM | 1113 | N | THR | A | 153 | 24.008 | 5.493 | 35.909 | 1.00 | 38.78 | N |
| ATOM | 1114 | CA | THR | A | 153 | 22.881 | 4.830 | 36.542 | 1.00 | 38.50 | C |
| ATOM | 1115 | C | THR | A | 153 | 21.757 | 4.573 | 35.573 | 1.00 | 38.26 | C |
| ATOM | 1116 | O | THR | A | 153 | 20.842 | 3.838 | 35.882 | 1.00 | 38.29 | O |
| ATOM | 1117 | CB | THR | A | 153 | 22.329 | 5.624 | 37.733 | 1.00 | 38.46 | C |
| ATOM | 1118 | OG1 | THR | A | 153 | 21.622 | 6.780 | 37.269 | 1.00 | 39.25 | O |
| ATOM | 1119 | CG2 | THR | A | 153 | 23.445 | 6.161 | 38.611 | 1.00 | 38.28 | C |
| ATOM | 1120 | N | VAL | A | 154 | 21.804 | 5.165 | 34.396 | 1.00 | 38.28 | N |
| ATOM | 1121 | CA | VAL | A | 154 | 20.687 | 4.977 | 33.491 | 1.00 | 38.29 | C |
| ATOM | 1122 | C | VAL | A | 154 | 20.602 | 3.530 | 33.067 | 1.00 | 38.17 | C |
| ATOM | 1123 | O | VAL | A | 154 | 21.597 | 2.805 | 33.092 | 1.00 | 38.10 | O |
| ATOM | 1124 | CB | VAL | A | 154 | 20.786 | 5.838 | 32.251 | 1.00 | 38.15 | C |
| ATOM | 1125 | CG1 | VAL | A | 154 | 20.815 | 7.291 | 32.649 | 1.00 | 38.22 | C |
| ATOM | 1126 | CG2 | VAL | A | 154 | 22.007 | 5.437 | 31.443 | 1.00 | 38.40 | C |
| ATOM | 1127 | N | GLY | A | 155 | 19.395 | 3.132 | 32.681 | 1.00 | 38.05 | N |
| ATOM | 1128 | CA | GLY | A | 155 | 19.114 | 1.779 | 32.258 | 1.00 | 38.07 | C |
| ATOM | 1129 | C | GLY | A | 155 | 19.609 | 1.358 | 30.894 | 1.00 | 38.17 | C |
| ATOM | 1130 | O | GLY | A | 155 | 20.092 | 2.153 | 30.081 | 1.00 | 38.44 | O |
| ATOM | 1131 | N | ARG | A | 156 | 19.417 | 0.073 | 30.642 | 1.00 | 38.16 | N |
| ATOM | 1132 | CA | ARG | A | 156 | 19.932 | -0.588 | 29.461 | 1.00 | 38.16 | C |
| ATOM | 1133 | C | ARG | A | 156 | 19.414 | 0.065 | 28.210 | 1.00 | 38.01 | C |
| ATOM | 1134 | O | ARG | A | 156 | 20.185 | 0.490 | 27.346 | 1.00 | 38.04 | O |
| ATOM | 1135 | CB | ARG | A | 156 | 19.554 | -2.080 | 29.489 | 1.00 | 38.18 | C |
| ATOM | 1136 | N | LYS | A | 157 | 18.102 | 0.178 | 28.118 | 1.00 | 37.83 | N |
| ATOM | 1137 | CA | LYS | A | 157 | 17.545 | 0.713 | 26.905 | 1.00 | 37.67 | C |
| ATOM | 1138 | C | LYS | A | 157 | 18.144 | 2.092 | 26.679 | 1.00 | 37.77 | C |
| ATOM | 1139 | O | LYS | A | 157 | 18.579 | 2.386 | 25.571 | 1.00 | 37.84 | O |
| ATOM | 1140 | CB | LYS | A | 157 | 16.014 | 0.725 | 26.936 | 1.00 | 37.62 | C |
| ATOM | 1141 | CG | LYS | A | 157 | 15.379 | -0.624 | 26.550 | 1.00 | 36.92 | C |
| ATOM | 1142 | N | ILE | A | 158 | 18.247 | 2.911 | 27.728 | 1.00 | 37.82 | N |
| ATOM | 1143 | CA | ILE | A | 158 | 18.699 | 4.287 | 27.526 | 1.00 | 37.81 | C |
| ATOM | 1144 | C | ILE | A | 158 | 20.096 | 4.252 | 27.008 | 1.00 | 37.78 | C |
| ATOM | 1145 | O | ILE | A | 158 | 20.440 | 4.942 | 26.058 | 1.00 | 37.52 | O |
| ATOM | 1146 | CB | ILE | A | 158 | 18.666 | 5.109 | 28.802 | 1.00 | 37.90 | C |
| ATOM | 1147 | CG1 | ILE | A | 158 | 17.233 | 5.283 | 29.280 | 1.00 | 37.87 | C |
| ATOM | 1148 | CG2 | ILE | A | 158 | 19.281 | 6.477 | 28.538 | 1.00 | 37.57 | C |
| ATOM | 1149 | CD1 | ILE | A | 158 | 16.383 | 6.034 | 28.318 | 1.00 | 37.95 | C |
| ATOM | 1150 | N | VAL | A | 159 | 20.899 | 3.418 | 27.637 | 1.00 | 37.89 | N |
| ATOM | 1151 | CA | VAL | A | 159 | 22.263 | 3.265 | 27.211 | 1.00 | 38.06 | C |
| ATOM | 1152 | C | VAL | A | 159 | 22.255 | 2.906 | 25.725 | 1.00 | 38.07 | C |
| ATOM | 1153 | O | VAL | A | 159 | 23.025 | 3.462 | 24.955 | 1.00 | 37.93 | O |
| ATOM | 1154 | CB | VAL | A | 159 | 22.987 | 2.196 | 28.039 | 1.00 | 38.12 | C |
| ATOM | 1155 | CG1 | VAL | A | 159 | 24.208 | 1.740 | 27.315 | 1.00 | 38.65 | C |
| ATOM | 1156 | CG2 | VAL | A | 159 | 23.368 | 2.734 | 29.410 | 1.00 | 37.65 | C |
| ATOM | 1157 | N | MET | A | 160 | 21.385 | 1.984 | 25.318 | 1.00 | 38.30 | N |
| ATOM | 1158 | CA | MET | A | 160 | 21.264 | 1.658 | 23.894 | 1.00 | 38.71 | C |
| ATOM | 1159 | C | MET | A | 160 | 21.024 | 2.923 | 23.084 | 1.00 | 38.35 | C |
| ATOM | 1160 | O | MET | A | 160 | 21.742 | 3.219 | 22.137 | 1.00 | 38.42 | O |
| ATOM | 1161 | CB | MET | A | 160 | 20.115 | 0.682 | 23.636 | 1.00 | 38.93 | C |
| ATOM | 1162 | CG | MET | A | 160 | 20.431 | -0.690 | 24.087 | 1.00 | 40.64 | C |
| ATOM | 1163 | SD | MET | A | 160 | 21.840 | -1.293 | 23.180 | 1.00 | 44.02 | S |
| ATOM | 1164 | CE | MET | A | 160 | 20.982 | -1.709 | 21.617 | 1.00 | 44.00 | C |
| ATOM | 1165 | N | ASP | A | 161 | 19.997 | 3.665 | 23.458 | 1.00 | 37.94 | N |
| ATOM | 1166 | CA | ASP | A | 161 | 19.702 | 4.902 | 22.773 | 1.00 | 37.82 | C |
| ATOM | 1167 | C | ASP | A | 161 | 20.955 | 5.788 | 22.684 | 1.00 | 37.50 | C |
| ATOM | 1168 | O | ASP | A | 161 | 21.395 | 6.154 | 21.596 | 1.00 | 37.66 | O |
| ATOM | 1169 | CB | ASP | A | 161 | 18.591 | 5.650 | 23.511 | 1.00 | 37.84 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1170 | CG | ASP | A | 161 | 17.274 | 4.908 | 23.501 | 1.00 | 37.82 | C |
| ATOM | 1171 | OD1 | ASP | A | 161 | 17.082 | 4.020 | 22.646 | 1.00 | 37.72 | O |
| ATOM | 1172 | OD2 | ASP | A | 161 | 16.366 | 5.155 | 24.320 | 1.00 | 38.41 | O |
| ATOM | 1173 | N | PHE | A | 162 | 21.539 | 6.100 | 23.836 | 1.00 | 36.93 | N |
| ATOM | 1174 | CA | PHE | A | 162 | 22.672 | 7.020 | 23.919 | 1.00 | 36.54 | C |
| ATOM | 1175 | C | PHE | A | 162 | 23.760 | 6.604 | 22.960 | 1.00 | 36.03 | C |
| ATOM | 1176 | O | PHE | A | 162 | 24.375 | 7.446 | 22.304 | 1.00 | 36.06 | O |
| ATOM | 1177 | CB | PHE | A | 162 | 23.201 | 7.063 | 25.364 | 1.00 | 36.52 | C |
| ATOM | 1178 | CG | PHE | A | 162 | 24.386 | 7.974 | 25.576 | 1.00 | 36.64 | C |
| ATOM | 1179 | CD1 | PHE | A | 162 | 24.209 | 9.319 | 25.871 | 1.00 | 36.67 | C |
| ATOM | 1180 | CD2 | PHE | A | 162 | 25.682 | 7.467 | 25.540 | 1.00 | 37.81 | C |
| ATOM | 1181 | CE1 | PHE | A | 162 | 25.299 | 10.155 | 26.081 | 1.00 | 36.91 | C |
| ATOM | 1182 | CE2 | PHE | A | 162 | 26.787 | 8.300 | 25.764 | 1.00 | 37.75 | C |
| ATOM | 1183 | CZ | PHE | A | 162 | 26.592 | 9.640 | 26.029 | 1.00 | 37.82 | C |
| ATOM | 1184 | N | LEU | A | 163 | 23.976 | 5.297 | 22.878 | 1.00 | 35.38 | N |
| ATOM | 1185 | CA | LEU | A | 163 | 24.998 | 4.730 | 22.023 | 1.00 | 34.93 | C |
| ATOM | 1186 | C | LEU | A | 163 | 24.635 | 4.948 | 20.591 | 1.00 | 34.41 | C |
| ATOM | 1187 | O | LEU | A | 163 | 25.502 | 5.067 | 19.732 | 1.00 | 34.36 | O |
| ATOM | 1188 | CB | LEU | A | 163 | 25.111 | 3.239 | 22.272 | 1.00 | 35.05 | C |
| ATOM | 1189 | CG | LEU | A | 163 | 25.977 | 2.932 | 23.473 | 1.00 | 35.25 | C |
| ATOM | 1190 | CD1 | LEU | A | 163 | 25.944 | 1.471 | 23.684 | 1.00 | 36.00 | C |
| ATOM | 1191 | CD2 | LEU | A | 163 | 27.404 | 3.425 | 23.270 | 1.00 | 35.64 | C |
| ATOM | 1192 | N | GLY | A | 164 | 23.336 | 4.977 | 20.338 | 1.00 | 33.85 | N |
| ATOM | 1193 | CA | GLY | A | 164 | 22.832 | 5.230 | 19.009 | 1.00 | 33.55 | C |
| ATOM | 1194 | C | GLY | A | 164 | 22.874 | 6.682 | 18.548 | 1.00 | 33.11 | C |
| ATOM | 1195 | O | GLY | A | 164 | 22.361 | 6.977 | 17.471 | 1.00 | 33.36 | O |
| ATOM | 1196 | N | PHE | A | 165 | 23.443 | 7.589 | 19.341 | 1.00 | 32.16 | N |
| ATOM | 1197 | CA | PHE | A | 165 | 23.593 | 8.964 | 18.894 | 1.00 | 31.85 | C |
| ATOM | 1198 | C | PHE | A | 165 | 24.628 | 8.972 | 17.752 | 1.00 | 30.93 | C |
| ATOM | 1199 | O | PHE | A | 165 | 25.413 | 8.063 | 17.650 | 1.00 | 30.67 | O |
| ATOM | 1200 | CB | PHE | A | 165 | 24.028 | 9.883 | 20.055 | 1.00 | 32.06 | C |
| ATOM | 1201 | CG | PHE | A | 165 | 22.989 | 10.052 | 21.160 | 1.00 | 32.55 | C |
| ATOM | 1202 | CD1 | PHE | A | 165 | 21.734 | 9.478 | 21.081 | 1.00 | 33.69 | C |
| ATOM | 1203 | CD2 | PHE | A | 165 | 23.293 | 10.786 | 22.289 | 1.00 | 32.64 | C |
| ATOM | 1204 | CE1 | PHE | A | 165 | 20.817 | 9.646 | 22.106 | 1.00 | 33.39 | C |
| ATOM | 1205 | CE2 | PHE | A | 165 | 22.380 | 10.948 | 23.308 | 1.00 | 32.11 | C |
| ATOM | 1206 | CZ | PHE | A | 165 | 21.150 | 10.380 | 23.218 | 1.00 | 32.69 | C |
| ATOM | 1207 | N | ASN | A | 166 | 24.600 | 9.977 | 16.881 | 1.00 | 30.43 | N |
| ATOM | 1208 | CA | ASN | A | 166 | 25.552 | 10.106 | 15.761 | 1.00 | 30.00 | C |
| ATOM | 1209 | C | ASN | A | 166 | 26.932 | 10.623 | 16.177 | 1.00 | 29.91 | C |
| ATOM | 1210 | O | ASN | A | 166 | 27.370 | 11.721 | 15.812 | 1.00 | 28.90 | O |
| ATOM | 1211 | CB | ASN | A | 166 | 24.957 | 11.013 | 14.673 | 1.00 | 29.86 | C |
| ATOM | 1212 | CG | ASN | A | 166 | 25.720 | 10.957 | 13.363 | 1.00 | 28.91 | C |
| ATOM | 1213 | OD1 | ASN | A | 166 | 26.836 | 10.423 | 13.282 | 1.00 | 27.68 | O |
| ATOM | 1214 | ND2 | ASN | A | 166 | 25.119 | 11.528 | 12.320 | 1.00 | 26.76 | N |
| ATOM | 1215 | N | TRP | A | 167 | 27.604 | 9.785 | 16.943 | 1.00 | 30.04 | N |
| ATOM | 1216 | CA | TRP | A | 167 | 28.938 | 10.044 | 17.399 | 1.00 | 30.41 | C |
| ATOM | 1217 | C | TRP | A | 167 | 29.823 | 10.295 | 16.205 | 1.00 | 30.80 | C |
| ATOM | 1218 | O | TRP | A | 167 | 30.708 | 11.141 | 16.237 | 1.00 | 30.55 | O |
| ATOM | 1219 | CB | TRP | A | 167 | 29.390 | 8.847 | 18.232 | 1.00 | 30.31 | C |
| ATOM | 1220 | CG | TRP | A | 167 | 28.513 | 8.746 | 19.433 | 1.00 | 30.59 | C |
| ATOM | 1221 | CD1 | TRP | A | 167 | 27.594 | 7.792 | 19.699 | 1.00 | 30.51 | C |
| ATOM | 1222 | CD2 | TRP | A | 167 | 28.422 | 9.696 | 20.502 | 1.00 | 31.94 | C |
| ATOM | 1223 | NE1 | TRP | A | 167 | 26.947 | 8.067 | 20.881 | 1.00 | 30.98 | N |
| ATOM | 1224 | CE2 | TRP | A | 167 | 27.442 | 9.232 | 21.395 | 1.00 | 31.41 | C |
| ATOM | 1225 | CE3 | TRP | A | 167 | 29.087 | 10.885 | 20.801 | 1.00 | 31.71 | C |
| ATOM | 1226 | CZ2 | TRP | A | 167 | 27.112 | 9.904 | 22.554 | 1.00 | 32.59 | C |
| ATOM | 1227 | CZ3 | TRP | A | 167 | 28.750 | 11.560 | 21.944 | 1.00 | 32.92 | C |
| ATOM | 1228 | CH2 | TRP | A | 167 | 27.773 | 11.072 | 22.811 | 1.00 | 33.34 | C |
| ATOM | 1229 | N | ASN | A | 168 | 29.549 | 9.596 | 15.119 | 1.00 | 31.69 | N |
| ATOM | 1230 | CA | ASN | A | 168 | 30.352 | 9.771 | 13.936 | 1.00 | 32.37 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1231 | C | ASN | A | 168 | 30.447 | 11.229 | 13.590 | 1.00 | 32.97 | C |
| ATOM | 1232 | O | ASN | A | 168 | 31.541 | 11.747 | 13.390 | 1.00 | 33.15 | O |
| ATOM | 1233 | CB | ASN | A | 168 | 29.729 | 9.064 | 12.749 | 1.00 | 32.68 | C |
| ATOM | 1234 | CG | ASN | A | 168 | 30.594 | 9.147 | 11.507 | 1.00 | 32.86 | C |
| ATOM | 1235 | OD1 | ASN | A | 168 | 31.797 | 8.914 | 11.574 | 1.00 | 35.02 | O |
| ATOM | 1236 | ND2 | ASN | A | 168 | 29.989 | 9.473 | 10.368 | 1.00 | 31.39 | N |
| ATOM | 1237 | N | TRP | A | 169 | 29.284 | 11.884 | 13.518 | 1.00 | 33.38 | N |
| ATOM | 1238 | CA | TRP | A | 169 | 29.200 | 13.279 | 13.107 | 1.00 | 33.28 | C |
| ATOM | 1239 | C | TRP | A | 169 | 29.711 | 14.237 | 14.149 | 1.00 | 33.33 | C |
| ATOM | 1240 | O | TRP | A | 169 | 30.406 | 15.188 | 13.834 | 1.00 | 33.43 | O |
| ATOM | 1241 | CB | TRP | A | 169 | 27.756 | 13.673 | 12.765 | 1.00 | 33.43 | C |
| ATOM | 1242 | CG | TRP | A | 169 | 27.618 | 15.134 | 12.412 | 1.00 | 33.11 | C |
| ATOM | 1243 | CD1 | TRP | A | 169 | 27.814 | 15.698 | 11.191 | 1.00 | 33.49 | C |
| ATOM | 1244 | CD2 | TRP | A | 169 | 27.293 | 16.205 | 13.294 | 1.00 | 32.94 | C |
| ATOM | 1245 | NE1 | TRP | A | 169 | 27.629 | 17.056 | 11.251 | 1.00 | 33.21 | N |
| ATOM | 1246 | CE2 | TRP | A | 169 | 27.306 | 17.397 | 12.533 | 1.00 | 33.42 | C |
| ATOM | 1247 | CE3 | TRP | A | 169 | 26.994 | 16.284 | 14.655 | 1.00 | 33.15 | C |
| ATOM | 1248 | CZ2 | TRP | A | 169 | 27.026 | 18.648 | 13.081 | 1.00 | 33.66 | C |
| ATOM | 1249 | CZ3 | TRP | A | 169 | 26.719 | 17.526 | 15.204 | 1.00 | 34.02 | C |
| ATOM | 1250 | CH2 | TRP | A | 169 | 26.733 | 18.695 | 14.413 | 1.00 | 34.21 | C |
| ATOM | 1251 | N | ILE | A | 170 | 29.369 | 14.021 | 15.398 | 1.00 | 33.54 | N |
| ATOM | 1252 | CA | ILE | A | 170 | 29.739 | 15.024 | 16.368 | 1.00 | 33.92 | C |
| ATOM | 1253 | C | ILE | A | 170 | 31.225 | 14.935 | 16.713 | 1.00 | 34.07 | C |
| ATOM | 1254 | O | ILE | A | 170 | 31.855 | 15.939 | 16.988 | 1.00 | 34.23 | O |
| ATOM | 1255 | CB | ILE | A | 170 | 28.832 | 14.947 | 17.591 | 1.00 | 33.84 | C |
| ATOM | 1256 | CG1 | ILE | A | 170 | 28.803 | 16.288 | 18.306 | 1.00 | 34.22 | C |
| ATOM | 1257 | CG2 | ILE | A | 170 | 29.295 | 13.858 | 18.499 | 1.00 | 34.45 | C |
| ATOM | 1258 | CD1 | ILE | A | 170 | 27.869 | 16.309 | 19.478 | 1.00 | 34.73 | C |
| ATOM | 1259 | N | ASN | A | 171 | 31.801 | 13.743 | 16.650 | 1.00 | 34.41 | N |
| ATOM | 1260 | CA | ASN | A | 171 | 33.222 | 13.593 | 16.950 | 1.00 | 34.46 | C |
| ATOM | 1261 | C | ASN | A | 171 | 34.055 | 14.322 | 15.918 | 1.00 | 34.56 | C |
| ATOM | 1262 | O | ASN | A | 171 | 35.055 | 14.949 | 16.260 | 1.00 | 34.66 | O |
| ATOM | 1263 | CB | ASN | A | 171 | 33.632 | 12.116 | 16.996 | 1.00 | 34.47 | C |
| ATOM | 1264 | CG | ASN | A | 171 | 32.969 | 11.356 | 18.128 | 1.00 | 33.99 | C |
| ATOM | 1265 | OD1 | ASN | A | 171 | 32.391 | 11.951 | 19.031 | 1.00 | 35.35 | O |
| ATOM | 1266 | ND2 | ASN | A | 171 | 33.040 | 10.036 | 18.077 | 1.00 | 32.53 | N |
| ATOM | 1267 | N | LYS | A | 172 | 33.652 | 14.217 | 14.654 | 1.00 | 34.75 | N |
| ATOM | 1268 | CA | LYS | A | 172 | 34.337 | 14.917 | 13.584 | 1.00 | 35.18 | C |
| ATOM | 1269 | C | LYS | A | 172 | 34.261 | 16.415 | 13.907 | 1.00 | 35.29 | C |
| ATOM | 1270 | O | LYS | A | 172 | 35.248 | 17.133 | 13.800 | 1.00 | 34.89 | O |
| ATOM | 1271 | CB | LYS | A | 172 | 33.711 | 14.600 | 12.216 | 1.00 | 35.26 | C |
| ATOM | 1272 | CG | LYS | A | 172 | 34.200 | 13.299 | 11.587 | 1.00 | 36.55 | C |
| ATOM | 1273 | CD | LYS | A | 172 | 33.873 | 13.158 | 10.090 | 1.00 | 38.20 | C |
| ATOM | 1274 | CE | LYS | A | 172 | 34.512 | 11.872 | 9.537 | 1.00 | 39.82 | C |
| ATOM | 1275 | NZ | LYS | A | 172 | 34.369 | 11.661 | 8.050 | 1.00 | 41.20 | N |
| ATOM | 1276 | N | GLN | A | 173 | 33.093 | 16.875 | 14.339 | 1.00 | 35.70 | N |
| ATOM | 1277 | CA | GLN | A | 173 | 32.931 | 18.272 | 14.699 | 1.00 | 36.20 | C |
| ATOM | 1278 | C | GLN | A | 173 | 33.929 | 18.633 | 15.771 | 1.00 | 36.47 | C |
| ATOM | 1279 | O | GLN | A | 173 | 34.605 | 19.656 | 15.686 | 1.00 | 36.97 | O |
| ATOM | 1280 | CB | GLN | A | 173 | 31.534 | 18.555 | 15.231 | 1.00 | 36.19 | C |
| ATOM | 1281 | CG | GLN | A | 173 | 30.473 | 18.637 | 14.167 | 1.00 | 36.97 | C |
| ATOM | 1282 | CD | GLN | A | 173 | 30.765 | 19.720 | 13.157 | 1.00 | 37.19 | C |
| ATOM | 1283 | OE1 | GLN | A | 173 | 31.198 | 20.808 | 13.531 | 1.00 | 38.68 | O |
| ATOM | 1284 | NE2 | GLN | A | 173 | 30.551 | 19.425 | 11.879 | 1.00 | 35.94 | N |
| ATOM | 1285 | N | GLN | A | 174 | 34.000 | 17.806 | 16.802 | 1.00 | 36.38 | N |
| ATOM | 1286 | CA | GLN | A | 174 | 34.945 | 18.041 | 17.866 | 1.00 | 36.42 | C |
| ATOM | 1287 | C | GLN | A | 174 | 36.360 | 18.102 | 17.283 | 1.00 | 36.56 | C |
| ATOM | 1288 | O | GLN | A | 174 | 37.161 | 18.945 | 17.672 | 1.00 | 36.42 | O |
| ATOM | 1289 | CB | GLN | A | 174 | 34.815 | 16.937 | 18.912 | 1.00 | 36.33 | C |
| ATOM | 1290 | CG | GLN | A | 174 | 35.896 | 16.908 | 19.963 | 1.00 | 36.13 | C |
| ATOM | 1291 | CD | GLN | A | 174 | 35.785 | 15.676 | 20.815 | 1.00 | 36.16 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1292 | OE1 | GLN | A | 174 | 35.415 | 14.613 | 20.314 | 1.00 | 37.84 | O |
| ATOM | 1293 | NE2 | GLN | A | 174 | 36.082 | 15.803 | 22.103 | 1.00 | 34.98 | N |
| ATOM | 1294 | N | GLY | A | 175 | 36.649 | 17.231 | 16.322 | 1.00 | 36.76 | N |
| ATOM | 1295 | CA | GLY | A | 175 | 37.976 | 17.158 | 15.750 | 1.00 | 36.97 | C |
| ATOM | 1296 | C | GLY | A | 175 | 38.302 | 18.356 | 14.892 | 1.00 | 37.21 | C |
| ATOM | 1297 | O | GLY | A | 175 | 39.336 | 18.993 | 15.070 | 1.00 | 37.38 | O |
| ATOM | 1298 | N | LYS | A | 176 | 37.406 | 18.682 | 13.971 | 1.00 | 37.44 | N |
| ATOM | 1299 | CA | LYS | A | 176 | 37.634 | 19.793 | 13.064 | 1.00 | 37.56 | C |
| ATOM | 1300 | C | LYS | A | 176 | 37.898 | 21.090 | 13.822 | 1.00 | 37.47 | C |
| ATOM | 1301 | O | LYS | A | 176 | 38.713 | 21.907 | 13.400 | 1.00 | 37.47 | O |
| ATOM | 1302 | CB | LYS | A | 176 | 36.423 | 20.014 | 12.161 | 1.00 | 37.71 | C |
| ATOM | 1303 | CG | LYS | A | 176 | 36.134 | 18.905 | 11.163 | 1.00 | 38.70 | C |
| ATOM | 1304 | CD | LYS | A | 176 | 34.960 | 19.284 | 10.279 | 1.00 | 39.76 | C |
| ATOM | 1305 | CE | LYS | A | 176 | 34.064 | 18.092 | 10.037 | 1.00 | 41.48 | C |
| ATOM | 1306 | NZ | LYS | A | 176 | 32.663 | 18.481 | 9.690 | 1.00 | 43.43 | N |
| ATOM | 1307 | N | ARG | A | 177 | 37.212 | 21.283 | 14.938 | 1.00 | 37.10 | N |
| ATOM | 1308 | CA | ARG | A | 177 | 37.325 | 22.544 | 15.643 | 1.00 | 37.08 | C |
| ATOM | 1309 | C | ARG | A | 177 | 38.352 | 22.495 | 16.763 | 1.00 | 36.85 | C |
| ATOM | 1310 | O | ARG | A | 177 | 38.445 | 23.420 | 17.564 | 1.00 | 36.21 | O |
| ATOM | 1311 | CB | ARG | A | 177 | 35.980 | 22.969 | 16.228 | 1.00 | 37.21 | C |
| ATOM | 1312 | CG | ARG | A | 177 | 34.807 | 22.773 | 15.326 | 1.00 | 37.50 | C |
| ATOM | 1313 | CD | ARG | A | 177 | 34.802 | 23.591 | 14.053 | 1.00 | 38.49 | C |
| ATOM | 1314 | NE | ARG | A | 177 | 33.750 | 23.066 | 13.185 | 1.00 | 39.56 | N |
| ATOM | 1315 | CZ | ARG | A | 177 | 33.884 | 22.803 | 11.891 | 1.00 | 41.17 | C |
| ATOM | 1316 | NH1 | ARG | A | 177 | 35.026 | 23.050 | 11.254 | 1.00 | 41.34 | N |
| ATOM | 1317 | NH2 | ARG | A | 177 | 32.855 | 22.304 | 11.219 | 1.00 | 41.89 | N |
| ATOM | 1318 | N | GLY | A | 178 | 39.088 | 21.401 | 16.859 | 1.00 | 36.70 | N |
| ATOM | 1319 | CA | GLY | A | 178 | 40.131 | 21.337 | 17.854 | 1.00 | 36.74 | C |
| ATOM | 1320 | C | GLY | A | 178 | 39.592 | 21.509 | 19.249 | 1.00 | 36.76 | C |
| ATOM | 1321 | O | GLY | A | 178 | 40.340 | 21.817 | 20.171 | 1.00 | 37.18 | O |
| ATOM | 1322 | N | TRP | A | 179 | 38.293 | 21.331 | 19.420 | 1.00 | 36.75 | N |
| ATOM | 1323 | CA | TRP | A | 179 | 37.722 | 21.439 | 20.745 | 1.00 | 36.66 | C |
| ATOM | 1324 | C | TRP | A | 179 | 38.309 | 20.400 | 21.679 | 1.00 | 36.60 | C |
| ATOM | 1325 | O | TRP | A | 179 | 38.980 | 19.451 | 21.260 | 1.00 | 35.99 | O |
| ATOM | 1326 | CB | TRP | A | 179 | 36.222 | 21.216 | 20.708 | 1.00 | 36.79 | C |
| ATOM | 1327 | CG | TRP | A | 179 | 35.454 | 22.258 | 20.038 | 1.00 | 36.51 | C |
| ATOM | 1328 | CD1 | TRP | A | 179 | 35.889 | 23.470 | 19.620 | 1.00 | 36.67 | C |
| ATOM | 1329 | CD2 | TRP | A | 179 | 34.081 | 22.180 | 19.692 | 1.00 | 37.40 | C |
| ATOM | 1330 | NE1 | TRP | A | 179 | 34.860 | 24.168 | 19.035 | 1.00 | 36.91 | N |
| ATOM | 1331 | CE2 | TRP | A | 179 | 33.735 | 23.390 | 19.062 | 1.00 | 37.43 | C |
| ATOM | 1332 | CE3 | TRP | A | 179 | 33.099 | 21.198 | 19.840 | 1.00 | 36.64 | C |
| ATOM | 1333 | CZ2 | TRP | A | 179 | 32.456 | 23.641 | 18.583 | 1.00 | 36.83 | C |
| ATOM | 1334 | CZ3 | TRP | A | 179 | 31.840 | 21.450 | 19.365 | 1.00 | 36.84 | C |
| ATOM | 1335 | CH2 | TRP | A | 179 | 31.524 | 22.661 | 18.744 | 1.00 | 36.02 | C |
| ATOM | 1336 | N | GLY | A | 180 | 38.022 | 20.595 | 22.958 | 1.00 | 36.66 | N |
| ATOM | 1337 | CA | GLY | A | 180 | 38.444 | 19.681 | 23.992 | 1.00 | 36.96 | C |
| ATOM | 1338 | C | GLY | A | 180 | 37.456 | 18.548 | 24.131 | 1.00 | 37.25 | C |
| ATOM | 1339 | O | GLY | A | 180 | 36.698 | 18.285 | 23.204 | 1.00 | 37.69 | O |
| ATOM | 1340 | N | GLN | A | 181 | 37.445 | 17.891 | 25.288 | 1.00 | 37.46 | N |
| ATOM | 1341 | CA | GLN | A | 181 | 36.581 | 16.734 | 25.507 | 1.00 | 37.81 | C |
| ATOM | 1342 | C | GLN | A | 181 | 35.136 | 17.088 | 25.802 | 1.00 | 37.40 | C |
| ATOM | 1343 | O | GLN | A | 181 | 34.825 | 18.177 | 26.273 | 1.00 | 37.59 | O |
| ATOM | 1344 | CB | GLN | A | 181 | 37.082 | 15.881 | 26.680 | 1.00 | 38.18 | C |
| ATOM | 1345 | CG | GLN | A | 181 | 36.684 | 16.433 | 28.065 | 1.00 | 40.32 | C |
| ATOM | 1346 | CD | GLN | A | 181 | 36.956 | 15.470 | 29.231 | 1.00 | 43.44 | C |
| ATOM | 1347 | OE1 | GLN | A | 181 | 38.004 | 14.802 | 29.284 | 1.00 | 44.84 | O |
| ATOM | 1348 | NE2 | GLN | A | 181 | 36.007 | 15.406 | 30.173 | 1.00 | 44.80 | N |
| ATOM | 1349 | N | LEU | A | 182 | 34.266 | 16.130 | 25.510 | 1.00 | 37.00 | N |
| ATOM | 1350 | CA | LEU | A | 182 | 32.866 | 16.181 | 25.878 | 1.00 | 36.47 | C |
| ATOM | 1351 | C | LEU | A | 182 | 32.856 | 16.224 | 27.385 | 1.00 | 35.97 | C |
| ATOM | 1352 | O | LEU | A | 182 | 33.345 | 15.298 | 28.009 | 1.00 | 35.98 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1353 | CB | LEU | A | 182 | 32.208 | 14.865 | 25.468 | 1.00 | 36.38 | C |
| ATOM | 1354 | CG | LEU | A | 182 | 30.691 | 14.707 | 25.336 | 1.00 | 36.76 | C |
| ATOM | 1355 | CD1 | LEU | A | 182 | 30.339 | 13.254 | 25.433 | 1.00 | 36.70 | C |
| ATOM | 1356 | CD2 | LEU | A | 182 | 29.917 | 15.417 | 26.376 | 1.00 | 37.66 | C |
| ATOM | 1357 | N | THR | A | 183 | 32.337 | 17.270 | 28.005 | 1.00 | 35.50 | N |
| ATOM | 1358 | CA | THR | A | 183 | 32.310 | 17.230 | 29.457 | 1.00 | 35.07 | C |
| ATOM | 1359 | C | THR | A | 183 | 31.008 | 16.669 | 29.929 | 1.00 | 34.39 | C |
| ATOM | 1360 | O | THR | A | 183 | 30.944 | 16.097 | 31.000 | 1.00 | 34.13 | O |
| ATOM | 1361 | CB | THR | A | 183 | 32.528 | 18.599 | 30.105 | 1.00 | 35.07 | C |
| ATOM | 1362 | OG1 | THR | A | 183 | 31.402 | 19.444 | 29.883 | 1.00 | 35.21 | O |
| ATOM | 1363 | CG2 | THR | A | 183 | 33.652 | 19.310 | 29.453 | 1.00 | 35.76 | C |
| ATOM | 1364 | N | SER | A | 184 | 29.947 | 16.848 | 29.163 | 1.00 | 33.83 | N |
| ATOM | 1365 | CA | SER | A | 184 | 28.710 | 16.288 | 29.626 | 1.00 | 33.19 | C |
| ATOM | 1366 | C | SER | A | 184 | 27.563 | 16.459 | 28.684 | 1.00 | 32.72 | C |
| ATOM | 1367 | O | SER | A | 184 | 27.643 | 17.172 | 27.699 | 1.00 | 32.59 | O |
| ATOM | 1368 | CB | SER | A | 184 | 28.363 | 16.954 | 30.949 | 1.00 | 33.18 | C |
| ATOM | 1369 | OG | SER | A | 184 | 28.349 | 18.347 | 30.788 | 1.00 | 31.82 | O |
| ATOM | 1370 | N | ASN | A | 185 | 26.484 | 15.776 | 29.013 | 1.00 | 32.44 | N |
| ATOM | 1371 | CA | ASN | A | 185 | 25.259 | 15.893 | 28.277 | 1.00 | 32.59 | C |
| ATOM | 1372 | C | ASN | A | 185 | 24.218 | 16.117 | 29.319 | 1.00 | 33.00 | C |
| ATOM | 1373 | O | ASN | A | 185 | 24.027 | 15.285 | 30.184 | 1.00 | 32.72 | O |
| ATOM | 1374 | CB | ASN | A | 185 | 24.917 | 14.619 | 27.520 | 1.00 | 32.46 | C |
| ATOM | 1375 | CG | ASN | A | 185 | 25.850 | 14.351 | 26.369 | 1.00 | 31.69 | C |
| ATOM | 1376 | OD1 | ASN | A | 185 | 26.661 | 13.436 | 26.434 | 1.00 | 32.60 | O |
| ATOM | 1377 | ND2 | ASN | A | 185 | 25.725 | 15.121 | 25.297 | 1.00 | 29.86 | N |
| ATOM | 1378 | N | LEU | A | 186 | 23.549 | 17.252 | 29.258 | 1.00 | 33.80 | N |
| ATOM | 1379 | CA | LEU | A | 186 | 22.537 | 17.536 | 30.241 | 1.00 | 34.36 | C |
| ATOM | 1380 | C | LEU | A | 186 | 21.199 | 17.117 | 29.684 | 1.00 | 34.78 | C |
| ATOM | 1381 | O | LEU | A | 186 | 20.903 | 17.380 | 28.512 | 1.00 | 35.02 | O |
| ATOM | 1382 | CB | LEU | A | 186 | 22.500 | 19.029 | 30.539 | 1.00 | 34.34 | C |
| ATOM | 1383 | CG | LEU | A | 186 | 21.564 | 19.433 | 31.677 | 1.00 | 35.25 | C |
| ATOM | 1384 | CD1 | LEU | A | 186 | 22.122 | 18.827 | 32.930 | 1.00 | 35.58 | C |
| ATOM | 1385 | CD2 | LEU | A | 186 | 21.402 | 20.956 | 31.845 | 1.00 | 35.43 | C |
| ATOM | 1386 | N | LEU | A | 187 | 20.393 | 16.456 | 30.507 | 1.00 | 34.95 | N |
| ATOM | 1387 | CA | LEU | A | 187 | 19.022 | 16.189 | 30.120 | 1.00 | 35.27 | C |
| ATOM | 1388 | C | LEU | A | 187 | 18.117 | 17.260 | 30.735 | 1.00 | 35.48 | C |
| ATOM | 1389 | O | LEU | A | 187 | 18.105 | 17.449 | 31.951 | 1.00 | 35.40 | O |
| ATOM | 1390 | CB | LEU | A | 187 | 18.593 | 14.805 | 30.563 | 1.00 | 35.33 | C |
| ATOM | 1391 | CG | LEU | A | 187 | 17.105 | 14.481 | 30.399 | 1.00 | 36.09 | C |
| ATOM | 1392 | CD1 | LEU | A | 187 | 16.624 | 14.525 | 28.969 | 1.00 | 36.40 | C |
| ATOM | 1393 | CD2 | LEU | A | 187 | 16.850 | 13.114 | 30.940 | 1.00 | 36.96 | C |
| ATOM | 1394 | N | LEU | A | 188 | 17.380 | 17.977 | 29.889 | 1.00 | 35.70 | N |
| ATOM | 1395 | CA | LEU | A | 188 | 16.466 | 19.005 | 30.362 | 1.00 | 35.89 | C |
| ATOM | 1396 | C | LEU | A | 188 | 15.047 | 18.668 | 29.972 | 1.00 | 36.32 | C |
| ATOM | 1397 | O | LEU | A | 188 | 14.738 | 18.548 | 28.792 | 1.00 | 36.89 | O |
| ATOM | 1398 | CB | LEU | A | 188 | 16.795 | 20.362 | 29.771 | 1.00 | 35.79 | C |
| ATOM | 1399 | CG | LEU | A | 188 | 18.210 | 20.889 | 29.937 | 1.00 | 35.66 | C |
| ATOM | 1400 | CD1 | LEU | A | 188 | 18.976 | 20.745 | 28.668 | 1.00 | 36.04 | C |
| ATOM | 1401 | CD2 | LEU | A | 188 | 18.125 | 22.328 | 30.284 | 1.00 | 35.23 | C |
| ATOM | 1402 | N | ILE | A | 189 | 14.184 | 18.514 | 30.967 | 1.00 | 36.45 | N |
| ATOM | 1403 | CA | ILE | A | 189 | 12.782 | 18.254 | 30.720 | 1.00 | 36.25 | C |
| ATOM | 1404 | C | ILE | A | 189 | 12.105 | 19.353 | 31.472 | 1.00 | 35.88 | C |
| ATOM | 1405 | O | ILE | A | 189 | 12.388 | 19.542 | 32.651 | 1.00 | 35.75 | O |
| ATOM | 1406 | CB | ILE | A | 189 | 12.368 | 16.916 | 31.274 | 1.00 | 36.47 | C |
| ATOM | 1407 | CG1 | ILE | A | 189 | 13.126 | 15.813 | 30.549 | 1.00 | 36.63 | C |
| ATOM | 1408 | CG2 | ILE | A | 189 | 10.865 | 16.748 | 31.143 | 1.00 | 36.55 | C |
| ATOM | 1409 | CD1 | ILE | A | 189 | 12.884 | 14.440 | 31.129 | 1.00 | 36.11 | C |
| ATOM | 1410 | N | GLY | A | 190 | 11.221 | 20.071 | 30.789 | 1.00 | 35.53 | N |
| ATOM | 1411 | CA | GLY | A | 190 | 10.614 | 21.257 | 31.344 | 1.00 | 35.37 | C |
| ATOM | 1412 | C | GLY | A | 190 | 9.184 | 21.420 | 30.921 | 1.00 | 35.23 | C |
| ATOM | 1413 | O | GLY | A | 190 | 8.748 | 20.857 | 29.930 | 1.00 | 35.26 | O |

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ATOM   1414  N   MET A 191      8.458  22.208  31.696  1.00 35.18           N
ATOM   1415  CA  MET A 191      7.063  22.463  31.447  1.00 35.16           C
ATOM   1416  C   MET A 191      6.916  23.584  30.446  1.00 35.00           C
ATOM   1417  O   MET A 191      7.795  24.426  30.316  1.00 35.17           O
ATOM   1418  CB  MET A 191      6.379  22.849  32.750  1.00 35.13           C
ATOM   1419  CG  MET A 191      6.277  21.691  33.710  1.00 35.63           C
ATOM   1420  SD  MET A 191      5.756  22.150  35.360  1.00 35.65           S
ATOM   1421  CE  MET A 191      4.222  22.827  35.017  1.00 36.16           C
ATOM   1422  N   GLU A 192      5.804  23.573  29.727  1.00 34.83           N
ATOM   1423  CA  GLU A 192      5.492  24.626  28.791  1.00 34.74           C
ATOM   1424  C   GLU A 192      5.585  25.955  29.511  1.00 34.72           C
ATOM   1425  O   GLU A 192      5.184  26.067  30.674  1.00 34.67           O
ATOM   1426  CB  GLU A 192      4.085  24.447  28.264  1.00 34.75           C
ATOM   1427  CG  GLU A 192      3.029  24.525  29.348  1.00 35.09           C
ATOM   1428  CD  GLU A 192      1.669  24.117  28.842  1.00 34.97           C
ATOM   1429  OE1 GLU A 192      1.609  23.503  27.756  1.00 33.58           O
ATOM   1430  OE2 GLU A 192      0.672  24.422  29.530  1.00 35.72           O
ATOM   1431  N   GLY A 193      6.121  26.953  28.818  1.00 34.53           N
ATOM   1432  CA  GLY A 193      6.265  28.279  29.378  1.00 34.63           C
ATOM   1433  C   GLY A 193      7.528  28.542  30.180  1.00 34.49           C
ATOM   1434  O   GLY A 193      7.864  29.694  30.434  1.00 34.57           O
ATOM   1435  N   ASN A 194      8.224  27.493  30.594  1.00 34.27           N
ATOM   1436  CA  ASN A 194      9.441  27.672  31.367  1.00 34.06           C
ATOM   1437  C   ASN A 194     10.466  28.492  30.609  1.00 33.93           C
ATOM   1438  O   ASN A 194     10.552  28.415  29.392  1.00 33.84           O
ATOM   1439  CB  ASN A 194     10.051  26.316  31.721  1.00 33.99           C
ATOM   1440  CG  ASN A 194      9.314  25.625  32.836  1.00 33.19           C
ATOM   1441  OD1 ASN A 194      8.257  26.081  33.265  1.00 33.07           O
ATOM   1442  ND2 ASN A 194      9.869  24.528  33.323  1.00 31.93           N
ATOM   1443  N   VAL A 195     11.243  29.285  31.332  1.00 33.86           N
ATOM   1444  CA  VAL A 195     12.288  30.069  30.707  1.00 33.70           C
ATOM   1445  C   VAL A 195     13.621  29.969  31.396  1.00 33.38           C
ATOM   1446  O   VAL A 195     13.721  30.115  32.601  1.00 33.75           O
ATOM   1447  CB  VAL A 195     11.964  31.552  30.779  1.00 33.96           C
ATOM   1448  CG1 VAL A 195     13.151  32.389  30.253  1.00 34.32           C
ATOM   1449  CG2 VAL A 195     10.693  31.854  30.032  1.00 34.15           C
ATOM   1450  N   THR A 196     14.666  29.764  30.621  1.00 33.04           N
ATOM   1451  CA  THR A 196     15.991  29.883  31.161  1.00 32.60           C
ATOM   1452  C   THR A 196     16.438  31.256  30.723  1.00 32.21           C
ATOM   1453  O   THR A 196     16.584  31.500  29.530  1.00 31.64           O
ATOM   1454  CB  THR A 196     16.887  28.836  30.586  1.00 32.68           C
ATOM   1455  OG1 THR A 196     16.466  27.543  31.048  1.00 33.09           O
ATOM   1456  CG2 THR A 196     18.281  29.003  31.124  1.00 32.63           C
ATOM   1457  N   PRO A 197     16.585  32.177  31.672  1.00 31.97           N
ATOM   1458  CA  PRO A 197     17.000  33.530  31.350  1.00 31.74           C
ATOM   1459  C   PRO A 197     18.385  33.564  30.816  1.00 31.92           C
ATOM   1460  O   PRO A 197     19.215  32.717  31.129  1.00 32.52           O
ATOM   1461  CB  PRO A 197     16.950  34.234  32.682  1.00 31.38           C
ATOM   1462  CG  PRO A 197     16.056  33.508  33.418  1.00 31.84           C
ATOM   1463  CD  PRO A 197     16.305  32.055  33.107  1.00 32.08           C
ATOM   1464  N   ALA A 198     18.615  34.592  30.024  1.00 32.06           N
ATOM   1465  CA  ALA A 198     19.846  34.787  29.311  1.00 32.28           C
ATOM   1466  C   ALA A 198     21.101  34.690  30.162  1.00 32.42           C
ATOM   1467  O   ALA A 198     21.213  35.305  31.220  1.00 32.03           O
ATOM   1468  CB  ALA A 198     19.798  36.131  28.625  1.00 32.42           C
ATOM   1469  N   HIS A 199     22.064  33.953  29.630  1.00 32.77           N
ATOM   1470  CA  HIS A 199     23.339  33.737  30.271  1.00 33.31           C
ATOM   1471  C   HIS A 199     24.308  33.252  29.220  1.00 33.76           C
ATOM   1472  O   HIS A 199     23.902  33.013  28.084  1.00 34.10           O
ATOM   1473  CB  HIS A 199     23.194  32.622  31.275  1.00 33.24           C
ATOM   1474  CG  HIS A 199     22.879  31.311  30.639  1.00 32.59           C
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ATOM   1475  ND1 HIS A 199      21.602  30.958  30.269  1.00 31.40           N
ATOM   1476  CD2 HIS A 199      23.679  30.292  30.253  1.00 32.85           C
ATOM   1477  CE1 HIS A 199      21.624  29.761  29.714  1.00 32.37           C
ATOM   1478  NE2 HIS A 199      22.871  29.330  29.698  1.00 32.78           N
ATOM   1479  N   TYR A 200      25.575  33.093  29.601  1.00 34.35           N
ATOM   1480  CA  TYR A 200      26.580  32.502  28.712  1.00 34.92           C
ATOM   1481  C   TYR A 200      27.256  31.350  29.431  1.00 35.15           C
ATOM   1482  O   TYR A 200      27.285  31.318  30.661  1.00 35.76           O
ATOM   1483  CB  TYR A 200      27.599  33.510  28.175  1.00 34.90           C
ATOM   1484  CG  TYR A 200      28.586  34.096  29.156  1.00 34.89           C
ATOM   1485  CD1 TYR A 200      29.825  33.519  29.359  1.00 33.02           C
ATOM   1486  CD2 TYR A 200      28.307  35.292  29.802  1.00 36.04           C
ATOM   1487  CE1 TYR A 200      30.731  34.079  30.224  1.00 33.25           C
ATOM   1488  CE2 TYR A 200      29.200  35.857  30.664  1.00 35.45           C
ATOM   1489  CZ  TYR A 200      30.410  35.253  30.882  1.00 34.40           C
ATOM   1490  OH  TYR A 200      31.301  35.855  31.739  1.00 32.62           O
ATOM   1491  N   ASP A 201      27.747  30.387  28.654  1.00 35.04           N
ATOM   1492  CA  ASP A 201      28.386  29.189  29.182  1.00 34.82           C
ATOM   1493  C   ASP A 201      29.818  29.220  28.652  1.00 34.87           C
ATOM   1494  O   ASP A 201      30.047  29.734  27.588  1.00 34.81           O
ATOM   1495  CB  ASP A 201      27.636  27.925  28.727  1.00 34.49           C
ATOM   1496  CG  ASP A 201      26.212  27.854  29.256  1.00 34.63           C
ATOM   1497  OD1 ASP A 201      26.046  27.953  30.480  1.00 33.52           O
ATOM   1498  OD2 ASP A 201      25.191  27.680  28.533  1.00 36.84           O
ATOM   1499  N   GLU A 202      30.795  28.727  29.399  1.00 35.74           N
ATOM   1500  CA  GLU A 202      32.176  28.699  28.899  1.00 36.38           C
ATOM   1501  C   GLU A 202      32.528  27.441  28.126  1.00 36.30           C
ATOM   1502  O   GLU A 202      33.679  27.019  28.126  1.00 37.04           O
ATOM   1503  CB  GLU A 202      33.172  28.830  30.048  1.00 36.61           C
ATOM   1504  CG  GLU A 202      33.100  30.185  30.725  1.00 37.81           C
ATOM   1505  CD  GLU A 202      33.960  30.276  31.949  1.00 38.93           C
ATOM   1506  OE1 GLU A 202      33.525  29.783  33.020  1.00 39.85           O
ATOM   1507  OE2 GLU A 202      35.055  30.858  31.832  1.00 40.19           O
ATOM   1508  N   GLN A 203      31.556  26.840  27.462  1.00 35.68           N
ATOM   1509  CA  GLN A 203      31.815  25.643  26.718  1.00 35.24           C
ATOM   1510  C   GLN A 203      31.107  25.754  25.406  1.00 34.57           C
ATOM   1511  O   GLN A 203      30.218  26.586  25.256  1.00 34.62           O
ATOM   1512  CB  GLN A 203      31.317  24.446  27.514  1.00 35.59           C
ATOM   1513  CG  GLN A 203      32.184  24.236  28.734  1.00 37.42           C
ATOM   1514  CD  GLN A 203      32.234  22.819  29.233  1.00 38.70           C
ATOM   1515  OE1 GLN A 203      32.228  21.860  28.458  1.00 39.80           O
ATOM   1516  NE2 GLN A 203      32.326  22.680  30.541  1.00 41.01           N
ATOM   1517  N   GLN A 204      31.524  24.939  24.443  1.00 33.68           N
ATOM   1518  CA  GLN A 204      30.873  24.899  23.165  1.00 32.97           C
ATOM   1519  C   GLN A 204      29.714  23.959  23.373  1.00 32.67           C
ATOM   1520  O   GLN A 204      29.838  22.982  24.082  1.00 32.33           O
ATOM   1521  CB  GLN A 204      31.793  24.352  22.093  1.00 32.85           C
ATOM   1522  CG  GLN A 204      33.042  25.165  21.819  1.00 32.50           C
ATOM   1523  CD  GLN A 204      32.786  26.454  21.057  1.00 30.59           C
ATOM   1524  OE1 GLN A 204      31.656  26.830  20.848  1.00 31.27           O
ATOM   1525  NE2 GLN A 204      33.843  27.132  20.664  1.00 29.18           N
ATOM   1526  N   ASN A 205      28.583  24.247  22.755  1.00 32.81           N
ATOM   1527  CA  ASN A 205      27.393  23.446  22.980  1.00 32.85           C
ATOM   1528  C   ASN A 205      26.594  23.059  21.733  1.00 32.80           C
ATOM   1529  O   ASN A 205      26.147  23.921  20.968  1.00 32.72           O
ATOM   1530  CB  ASN A 205      26.484  24.246  23.919  1.00 32.83           C
ATOM   1531  CG  ASN A 205      25.178  23.566  24.205  1.00 32.43           C
ATOM   1532  OD1 ASN A 205      24.914  22.465  23.732  1.00 32.78           O
ATOM   1533  ND2 ASN A 205      24.339  24.228  24.993  1.00 31.52           N
ATOM   1534  N   PHE A 206      26.427  21.763  21.515  1.00 32.36           N
ATOM   1535  CA  PHE A 206      25.454  21.326  20.541  1.00 32.02           C
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ATOM   1536  C   PHE A 206      24.167  20.977  21.301  1.00 31.59           C
ATOM   1537  O   PHE A 206      24.144  20.067  22.096  1.00 31.13           O
ATOM   1538  CB  PHE A 206      25.972  20.159  19.754  1.00 32.17           C
ATOM   1539  CG  PHE A 206      26.844  20.554  18.639  1.00 32.42           C
ATOM   1540  CD1 PHE A 206      26.364  21.354  17.630  1.00 33.16           C
ATOM   1541  CD2 PHE A 206      28.149  20.132  18.600  1.00 33.19           C
ATOM   1542  CE1 PHE A 206      27.174  21.721  16.600  1.00 33.34           C
ATOM   1543  CE2 PHE A 206      28.963  20.487  17.580  1.00 32.88           C
ATOM   1544  CZ  PHE A 206      28.485  21.279  16.574  1.00 33.50           C
ATOM   1545  N   PHE A 207      23.104  21.717  21.012  1.00 31.65           N
ATOM   1546  CA  PHE A 207      21.829  21.671  21.726  1.00 31.71           C
ATOM   1547  C   PHE A 207      20.822  20.825  20.924  1.00 31.35           C
ATOM   1548  O   PHE A 207      20.289  21.292  19.930  1.00 30.81           O
ATOM   1549  CB  PHE A 207      21.391  23.148  21.883  1.00 31.56           C
ATOM   1550  CG  PHE A 207      20.118  23.404  22.683  1.00 31.43           C
ATOM   1551  CD1 PHE A 207      18.926  23.676  22.036  1.00 32.30           C
ATOM   1552  CD2 PHE A 207      20.150  23.519  24.058  1.00 31.29           C
ATOM   1553  CE1 PHE A 207      17.781  23.982  22.748  1.00 32.37           C
ATOM   1554  CE2 PHE A 207      19.006  23.832  24.776  1.00 31.14           C
ATOM   1555  CZ  PHE A 207      17.828  24.062  24.122  1.00 32.27           C
ATOM   1556  N   ALA A 208      20.554  19.593  21.368  1.00 31.31           N
ATOM   1557  CA  ALA A 208      19.685  18.672  20.611  1.00 31.33           C
ATOM   1558  C   ALA A 208      18.264  18.543  21.138  1.00 31.59           C
ATOM   1559  O   ALA A 208      18.016  17.860  22.133  1.00 31.13           O
ATOM   1560  CB  ALA A 208      20.293  17.334  20.537  1.00 30.98           C
ATOM   1561  N   GLN A 209      17.340  19.169  20.409  1.00 32.00           N
ATOM   1562  CA  GLN A 209      15.935  19.183  20.751  1.00 32.37           C
ATOM   1563  C   GLN A 209      15.288  17.867  20.358  1.00 32.76           C
ATOM   1564  O   GLN A 209      15.492  17.360  19.247  1.00 32.19           O
ATOM   1565  CB  GLN A 209      15.245  20.332  20.031  1.00 32.55           C
ATOM   1566  CG  GLN A 209      13.802  20.589  20.470  1.00 32.44           C
ATOM   1567  CD  GLN A 209      13.689  20.978  21.925  1.00 32.27           C
ATOM   1568  OE1 GLN A 209      14.699  21.254  22.587  1.00 31.73           O
ATOM   1569  NE2 GLN A 209      12.457  21.000  22.436  1.00 32.63           N
ATOM   1570  N   ILE A 210      14.467  17.360  21.272  1.00 33.20           N
ATOM   1571  CA  ILE A 210      13.907  16.030  21.165  1.00 33.55           C
ATOM   1572  C   ILE A 210      12.399  15.998  21.195  1.00 33.37           C
ATOM   1573  O   ILE A 210      11.788  15.337  20.369  1.00 33.25           O
ATOM   1574  CB  ILE A 210      14.456  15.210  22.302  1.00 33.79           C
ATOM   1575  CG1 ILE A 210      15.900  14.837  21.980  1.00 34.71           C
ATOM   1576  CG2 ILE A 210      13.604  13.982  22.528  1.00 33.99           C
ATOM   1577  CD1 ILE A 210      16.679  14.375  23.191  1.00 35.48           C
ATOM   1578  N   LYS A 211      11.804  16.688  22.156  1.00 33.27           N
ATOM   1579  CA  LYS A 211      10.365  16.739  22.263  1.00 33.48           C
ATOM   1580  C   LYS A 211       9.960  18.146  22.559  1.00 33.68           C
ATOM   1581  O   LYS A 211      10.545  18.789  23.407  1.00 34.10           O
ATOM   1582  CB  LYS A 211       9.867  15.875  23.405  1.00 33.57           C
ATOM   1583  CG  LYS A 211       8.355  15.708  23.409  1.00 34.06           C
ATOM   1584  CD  LYS A 211       7.840  15.250  24.752  1.00 34.79           C
ATOM   1585  CE  LYS A 211       6.635  14.324  24.635  1.00 35.65           C
ATOM   1586  NZ  LYS A 211       5.876  14.398  23.369  1.00 36.67           N
ATOM   1587  N   GLY A 212       8.938  18.626  21.876  1.00 34.06           N
ATOM   1588  CA  GLY A 212       8.460  19.969  22.103  1.00 34.09           C
ATOM   1589  C   GLY A 212       9.270  20.966  21.314  1.00 34.27           C
ATOM   1590  O   GLY A 212      10.156  20.599  20.532  1.00 34.27           O
ATOM   1591  N   TYR A 213       8.955  22.237  21.523  1.00 34.23           N
ATOM   1592  CA  TYR A 213       9.640  23.311  20.843  1.00 34.12           C
ATOM   1593  C   TYR A 213      10.216  24.318  21.824  1.00 33.81           C
ATOM   1594  O   TYR A 213       9.602  24.652  22.835  1.00 33.09           O
ATOM   1595  CB  TYR A 213       8.665  23.994  19.899  1.00 34.42           C
ATOM   1596  CG  TYR A 213       8.257  23.091  18.789  1.00 35.40           C
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ATOM   1597  CD1 TYR A 213       7.228  22.163  18.955  1.00 36.80           C
ATOM   1598  CD2 TYR A 213       8.929  23.122  17.586  1.00 36.00           C
ATOM   1599  CE1 TYR A 213       6.873  21.323  17.944  1.00 36.82           C
ATOM   1600  CE2 TYR A 213       8.579  22.292  16.567  1.00 37.06           C
ATOM   1601  CZ  TYR A 213       7.560  21.390  16.743  1.00 37.82           C
ATOM   1602  OH  TYR A 213       7.242  20.568  15.688  1.00 40.76           O
ATOM   1603  N   LYS A 214      11.410  24.804  21.517  1.00 33.91           N
ATOM   1604  CA  LYS A 214      12.046  25.809  22.359  1.00 33.87           C
ATOM   1605  C   LYS A 214      12.479  27.033  21.551  1.00 33.71           C
ATOM   1606  O   LYS A 214      13.173  26.918  20.538  1.00 33.58           O
ATOM   1607  CB  LYS A 214      13.237  25.208  23.101  1.00 33.64           C
ATOM   1608  CG  LYS A 214      12.881  24.443  24.364  1.00 33.56           C
ATOM   1609  CD  LYS A 214      14.126  23.861  24.973  1.00 33.29           C
ATOM   1610  CE  LYS A 214      14.001  23.615  26.458  1.00 33.54           C
ATOM   1611  NZ  LYS A 214      15.346  23.419  27.130  1.00 32.27           N
ATOM   1612  N   ARG A 215      12.043  28.205  21.986  1.00 33.56           N
ATOM   1613  CA  ARG A 215      12.479  29.427  21.339  1.00 33.91           C
ATOM   1614  C   ARG A 215      13.816  29.800  21.944  1.00 33.54           C
ATOM   1615  O   ARG A 215      13.946  29.923  23.146  1.00 32.78           O
ATOM   1616  CB  ARG A 215      11.482  30.552  21.558  1.00 34.15           C
ATOM   1617  CG  ARG A 215      11.865  31.844  20.885  1.00 34.51           C
ATOM   1618  CD  ARG A 215      11.287  33.028  21.593  1.00 34.99           C
ATOM   1619  NE  ARG A 215      11.381  34.255  20.823  1.00 35.43           N
ATOM   1620  CZ  ARG A 215      10.688  35.346  21.103  1.00 35.27           C
ATOM   1621  NH1 ARG A 215       9.860  35.371  22.144  1.00 34.68           N
ATOM   1622  NH2 ARG A 215      10.829  36.415  20.344  1.00 35.16           N
ATOM   1623  N   CYS A 216      14.810  29.962  21.092  1.00 33.76           N
ATOM   1624  CA  CYS A 216      16.152  30.238  21.542  1.00 33.91           C
ATOM   1625  C   CYS A 216      16.555  31.613  21.068  1.00 34.31           C
ATOM   1626  O   CYS A 216      16.534  31.885  19.872  1.00 34.69           O
ATOM   1627  CB  CYS A 216      17.099  29.189  20.968  1.00 33.84           C
ATOM   1628  SG  CYS A 216      16.655  27.490  21.397  1.00 32.85           S
ATOM   1629  N   ILE A 217      16.886  32.494  22.004  1.00 34.57           N
ATOM   1630  CA  ILE A 217      17.335  33.830  21.648  1.00 34.82           C
ATOM   1631  C   ILE A 217      18.785  33.999  22.046  1.00 34.50           C
ATOM   1632  O   ILE A 217      19.136  33.839  23.213  1.00 34.30           O
ATOM   1633  CB  ILE A 217      16.475  34.890  22.324  1.00 35.07           C
ATOM   1634  CG1 ILE A 217      15.003  34.652  22.001  1.00 35.20           C
ATOM   1635  CG2 ILE A 217      16.881  36.259  21.844  1.00 35.38           C
ATOM   1636  CD1 ILE A 217      14.086  35.585  22.722  1.00 36.16           C
ATOM   1637  N   LEU A 218      19.620  34.315  21.060  1.00 34.32           N
ATOM   1638  CA  LEU A 218      21.052  34.443  21.277  1.00 34.44           C
ATOM   1639  C   LEU A 218      21.565  35.844  21.017  1.00 34.27           C
ATOM   1640  O   LEU A 218      21.074  36.561  20.148  1.00 34.59           O
ATOM   1641  CB  LEU A 218      21.818  33.476  20.365  1.00 34.57           C
ATOM   1642  CG  LEU A 218      21.953  32.036  20.844  1.00 34.62           C
ATOM   1643  CD1 LEU A 218      20.614  31.435  21.124  1.00 34.96           C
ATOM   1644  CD2 LEU A 218      22.638  31.235  19.789  1.00 35.31           C
ATOM   1645  N   PHE A 219      22.594  36.200  21.768  1.00 33.79           N
ATOM   1646  CA  PHE A 219      23.258  37.462  21.632  1.00 33.40           C
ATOM   1647  C   PHE A 219      24.730  37.155  21.617  1.00 33.29           C
ATOM   1648  O   PHE A 219      25.222  36.434  22.463  1.00 33.45           O
ATOM   1649  CB  PHE A 219      22.964  38.330  22.832  1.00 33.37           C
ATOM   1650  CG  PHE A 219      21.509  38.586  23.051  1.00 33.91           C
ATOM   1651  CD1 PHE A 219      20.852  39.607  22.379  1.00 33.73           C
ATOM   1652  CD2 PHE A 219      20.794  37.812  23.942  1.00 33.70           C
ATOM   1653  CE1 PHE A 219      19.512  39.832  22.600  1.00 33.52           C
ATOM   1654  CE2 PHE A 219      19.460  38.038  24.156  1.00 33.47           C
ATOM   1655  CZ  PHE A 219      18.818  39.045  23.486  1.00 33.23           C
ATOM   1656  N   PRO A 220      25.438  37.683  20.642  1.00 33.46           N
ATOM   1657  CA  PRO A 220      26.888  37.496  20.536  1.00 33.50           C
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1658 | C | PRO | A | 220 | 27.675 | 38.131 | 21.699 | 1.00 33.51 | C |
| ATOM | 1659 | O | PRO | A | 220 | 27.185 | 39.049 | 22.363 | 1.00 33.18 | O |
| ATOM | 1660 | CB | PRO | A | 220 | 27.246 | 38.169 | 19.211 | 1.00 33.51 | C |
| ATOM | 1661 | CG | PRO | A | 220 | 25.977 | 38.683 | 18.629 | 1.00 33.41 | C |
| ATOM | 1662 | CD | PRO | A | 220 | 24.869 | 38.462 | 19.544 | 1.00 33.33 | C |
| ATOM | 1663 | N | PRO | A | 221 | 28.886 | 37.627 | 21.942 | 1.00 33.38 | N |
| ATOM | 1664 | CA | PRO | A | 221 | 29.731 | 38.102 | 23.044 | 1.00 33.30 | C |
| ATOM | 1665 | C | PRO | A | 221 | 29.966 | 39.581 | 23.081 | 1.00 33.55 | C |
| ATOM | 1666 | O | PRO | A | 221 | 30.043 | 40.151 | 24.147 | 1.00 33.66 | O |
| ATOM | 1667 | CB | PRO | A | 221 | 31.033 | 37.375 | 22.799 | 1.00 33.11 | C |
| ATOM | 1668 | CG | PRO | A | 221 | 30.589 | 36.128 | 22.147 | 1.00 33.06 | C |
| ATOM | 1669 | CD | PRO | A | 221 | 29.523 | 36.522 | 21.207 | 1.00 32.91 | C |
| ATOM | 1670 | N | ASP | A | 222 | 30.009 | 40.217 | 21.933 | 1.00 34.30 | N |
| ATOM | 1671 | CA | ASP | A | 222 | 30.277 | 41.628 | 21.904 | 1.00 34.71 | C |
| ATOM | 1672 | C | ASP | A | 222 | 29.073 | 42.419 | 22.382 | 1.00 34.56 | C |
| ATOM | 1673 | O | ASP | A | 222 | 29.048 | 43.634 | 22.241 | 1.00 34.68 | O |
| ATOM | 1674 | CB | ASP | A | 222 | 30.679 | 42.055 | 20.502 | 1.00 34.79 | C |
| ATOM | 1675 | CG | ASP | A | 222 | 29.508 | 42.228 | 19.608 | 1.00 36.26 | C |
| ATOM | 1676 | OD1 | ASP | A | 222 | 28.387 | 41.897 | 20.028 | 1.00 38.21 | O |
| ATOM | 1677 | OD2 | ASP | A | 222 | 29.601 | 42.692 | 18.462 | 1.00 40.87 | O |
| ATOM | 1678 | N | GLN | A | 223 | 28.062 | 41.760 | 22.930 | 1.00 34.48 | N |
| ATOM | 1679 | CA | GLN | A | 223 | 26.965 | 42.532 | 23.497 | 1.00 34.78 | C |
| ATOM | 1680 | C | GLN | A | 223 | 27.031 | 42.541 | 25.011 | 1.00 34.33 | C |
| ATOM | 1681 | O | GLN | A | 223 | 26.077 | 42.878 | 25.686 | 1.00 34.70 | O |
| ATOM | 1682 | CB | GLN | A | 223 | 25.595 | 42.133 | 22.940 | 1.00 34.87 | C |
| ATOM | 1683 | CG | GLN | A | 223 | 25.364 | 42.825 | 21.599 | 1.00 36.55 | C |
| ATOM | 1684 | CD | GLN | A | 223 | 23.990 | 42.635 | 21.020 | 1.00 39.56 | C |
| ATOM | 1685 | OE1 | GLN | A | 223 | 22.986 | 42.824 | 21.701 | 1.00 42.40 | O |
| ATOM | 1686 | NE2 | GLN | A | 223 | 23.936 | 42.294 | 19.742 | 1.00 41.89 | N |
| ATOM | 1687 | N | PHE | A | 224 | 28.198 | 42.219 | 25.534 | 1.00 34.13 | N |
| ATOM | 1688 | CA | PHE | A | 224 | 28.437 | 42.270 | 26.965 | 1.00 34.17 | C |
| ATOM | 1689 | C | PHE | A | 224 | 27.941 | 43.571 | 27.570 | 1.00 34.88 | C |
| ATOM | 1690 | O | PHE | A | 224 | 27.310 | 43.549 | 28.622 | 1.00 35.50 | O |
| ATOM | 1691 | CB | PHE | A | 224 | 29.932 | 42.159 | 27.224 | 1.00 33.66 | C |
| ATOM | 1692 | CG | PHE | A | 224 | 30.305 | 42.027 | 28.661 | 1.00 32.69 | C |
| ATOM | 1693 | CD1 | PHE | A | 224 | 30.429 | 43.137 | 29.476 | 1.00 33.11 | C |
| ATOM | 1694 | CD2 | PHE | A | 224 | 30.609 | 40.790 | 29.191 | 1.00 31.85 | C |
| ATOM | 1695 | CE1 | PHE | A | 224 | 30.821 | 43.003 | 30.817 | 1.00 31.76 | C |
| ATOM | 1696 | CE2 | PHE | A | 224 | 30.993 | 40.661 | 30.498 | 1.00 31.29 | C |
| ATOM | 1697 | CZ | PHE | A | 224 | 31.098 | 41.775 | 31.316 | 1.00 30.73 | C |
| ATOM | 1698 | N | GLU | A | 225 | 28.235 | 44.706 | 26.930 | 1.00 35.46 | N |
| ATOM | 1699 | CA | GLU | A | 225 | 27.852 | 45.994 | 27.492 | 1.00 35.85 | C |
| ATOM | 1700 | C | GLU | A | 225 | 26.362 | 46.133 | 27.608 | 1.00 35.42 | C |
| ATOM | 1701 | O | GLU | A | 225 | 25.873 | 46.955 | 28.386 | 1.00 35.16 | O |
| ATOM | 1702 | CB | GLU | A | 225 | 28.401 | 47.175 | 26.688 | 1.00 36.59 | C |
| ATOM | 1703 | CG | GLU | A | 225 | 29.892 | 47.377 | 26.917 | 1.00 39.78 | C |
| ATOM | 1704 | CD | GLU | A | 225 | 30.357 | 48.822 | 27.125 | 1.00 43.65 | C |
| ATOM | 1705 | OE1 | GLU | A | 225 | 29.937 | 49.524 | 28.099 | 1.00 44.64 | O |
| ATOM | 1706 | OE2 | GLU | A | 225 | 31.224 | 49.234 | 26.319 | 1.00 47.74 | O |
| ATOM | 1707 | N | CYS | A | 226 | 25.633 | 45.329 | 26.851 | 1.00 35.07 | N |
| ATOM | 1708 | CA | CYS | A | 226 | 24.192 | 45.453 | 26.842 | 1.00 34.93 | C |
| ATOM | 1709 | C | CYS | A | 226 | 23.473 | 44.498 | 27.770 | 1.00 34.91 | C |
| ATOM | 1710 | O | CYS | A | 226 | 22.266 | 44.654 | 28.019 | 1.00 34.86 | O |
| ATOM | 1711 | CB | CYS | A | 226 | 23.681 | 45.196 | 25.448 | 1.00 34.80 | C |
| ATOM | 1712 | SG | CYS | A | 226 | 24.135 | 46.461 | 24.291 | 1.00 34.76 | S |
| ATOM | 1713 | N | LEU | A | 227 | 24.191 | 43.521 | 28.296 | 1.00 34.47 | N |
| ATOM | 1714 | CA | LEU | A | 227 | 23.509 | 42.483 | 29.025 | 1.00 34.57 | C |
| ATOM | 1715 | C | LEU | A | 227 | 23.815 | 42.408 | 30.503 | 1.00 34.08 | C |
| ATOM | 1716 | O | LEU | A | 227 | 23.122 | 41.725 | 31.235 | 1.00 33.57 | O |
| ATOM | 1717 | CB | LEU | A | 227 | 23.739 | 41.162 | 28.313 | 1.00 34.97 | C |
| ATOM | 1718 | CG | LEU | A | 227 | 22.883 | 41.127 | 27.047 | 1.00 36.04 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1719 | CD1 | LEU | A | 227 | 23.454 | 40.177 | 26.043 | 1.00 | 37.99 | C |
| ATOM | 1720 | CD2 | LEU | A | 227 | 21.474 | 40.719 | 27.394 | 1.00 | 36.66 | C |
| ATOM | 1721 | N | TYR | A | 228 | 24.866 | 43.104 | 30.917 | 1.00 | 34.23 | N |
| ATOM | 1722 | CA | TYR | A | 228 | 25.172 | 43.334 | 32.329 | 1.00 | 34.02 | C |
| ATOM | 1723 | C | TYR | A | 228 | 25.163 | 42.091 | 33.196 | 1.00 | 33.81 | C |
| ATOM | 1724 | O | TYR | A | 228 | 24.294 | 41.900 | 34.041 | 1.00 | 33.87 | O |
| ATOM | 1725 | CB | TYR | A | 228 | 24.183 | 44.345 | 32.897 | 1.00 | 33.73 | C |
| ATOM | 1726 | CG | TYR | A | 228 | 24.153 | 45.658 | 32.166 | 1.00 | 33.50 | C |
| ATOM | 1727 | CD1 | TYR | A | 228 | 24.947 | 46.712 | 32.568 | 1.00 | 33.63 | C |
| ATOM | 1728 | CD2 | TYR | A | 228 | 23.312 | 45.853 | 31.086 | 1.00 | 35.03 | C |
| ATOM | 1729 | CE1 | TYR | A | 228 | 24.903 | 47.932 | 31.924 | 1.00 | 34.25 | C |
| ATOM | 1730 | CE2 | TYR | A | 228 | 23.268 | 47.066 | 30.419 | 1.00 | 35.62 | C |
| ATOM | 1731 | CZ | TYR | A | 228 | 24.068 | 48.106 | 30.848 | 1.00 | 35.60 | C |
| ATOM | 1732 | OH | TYR | A | 228 | 24.027 | 49.324 | 30.203 | 1.00 | 36.79 | O |
| ATOM | 1733 | N | PRO | A | 229 | 26.170 | 41.263 | 33.027 | 1.00 | 33.75 | N |
| ATOM | 1734 | CA | PRO | A | 229 | 26.255 | 40.032 | 33.791 | 1.00 | 33.73 | C |
| ATOM | 1735 | C | PRO | A | 229 | 26.538 | 40.313 | 35.231 | 1.00 | 33.32 | C |
| ATOM | 1736 | O | PRO | A | 229 | 27.228 | 41.263 | 35.530 | 1.00 | 33.73 | O |
| ATOM | 1737 | CB | PRO | A | 229 | 27.449 | 39.319 | 33.169 | 1.00 | 33.87 | C |
| ATOM | 1738 | CG | PRO | A | 229 | 28.264 | 40.366 | 32.543 | 1.00 | 33.66 | C |
| ATOM | 1739 | CD | PRO | A | 229 | 27.334 | 41.457 | 32.156 | 1.00 | 34.15 | C |
| ATOM | 1740 | N | TYR | A | 230 | 25.992 | 39.509 | 36.122 | 1.00 | 32.95 | N |
| ATOM | 1741 | CA | TYR | A | 230 | 26.330 | 39.654 | 37.510 | 1.00 | 32.64 | C |
| ATOM | 1742 | C | TYR | A | 230 | 27.836 | 39.534 | 37.651 | 1.00 | 32.59 | C |
| ATOM | 1743 | O | TYR | A | 230 | 28.536 | 39.020 | 36.793 | 1.00 | 32.76 | O |
| ATOM | 1744 | CB | TYR | A | 230 | 25.713 | 38.547 | 38.351 | 1.00 | 32.25 | C |
| ATOM | 1745 | CG | TYR | A | 230 | 24.237 | 38.640 | 38.573 | 1.00 | 31.53 | C |
| ATOM | 1746 | CD1 | TYR | A | 230 | 23.346 | 38.125 | 37.641 | 1.00 | 31.07 | C |
| ATOM | 1747 | CD2 | TYR | A | 230 | 23.727 | 39.192 | 39.748 | 1.00 | 29.93 | C |
| ATOM | 1748 | CE1 | TYR | A | 230 | 21.996 | 38.185 | 37.859 | 1.00 | 31.19 | C |
| ATOM | 1749 | CE2 | TYR | A | 230 | 22.395 | 39.253 | 39.980 | 1.00 | 28.83 | C |
| ATOM | 1750 | CZ | TYR | A | 230 | 21.523 | 38.755 | 39.040 | 1.00 | 31.04 | C |
| ATOM | 1751 | OH | TYR | A | 230 | 20.165 | 38.816 | 39.272 | 1.00 | 32.40 | O |
| ATOM | 1752 | N | PRO | A | 231 | 28.328 | 40.016 | 38.764 | 1.00 | 32.69 | N |
| ATOM | 1753 | CA | PRO | A | 231 | 29.725 | 39.852 | 39.124 | 1.00 | 32.75 | C |
| ATOM | 1754 | C | PRO | A | 231 | 30.159 | 38.384 | 39.159 | 1.00 | 32.72 | C |
| ATOM | 1755 | O | PRO | A | 231 | 29.434 | 37.497 | 39.604 | 1.00 | 32.86 | O |
| ATOM | 1756 | CB | PRO | A | 231 | 29.768 | 40.423 | 40.533 | 1.00 | 32.82 | C |
| ATOM | 1757 | CG | PRO | A | 231 | 28.625 | 41.349 | 40.605 | 1.00 | 32.96 | C |
| ATOM | 1758 | CD | PRO | A | 231 | 27.576 | 40.802 | 39.751 | 1.00 | 32.88 | C |
| ATOM | 1759 | N | VAL | A | 232 | 31.387 | 38.151 | 38.740 | 1.00 | 32.40 | N |
| ATOM | 1760 | CA | VAL | A | 232 | 31.938 | 36.825 | 38.680 | 1.00 | 32.10 | C |
| ATOM | 1761 | C | VAL | A | 232 | 31.776 | 36.022 | 39.963 | 1.00 | 32.41 | C |
| ATOM | 1762 | O | VAL | A | 232 | 31.546 | 34.826 | 39.906 | 1.00 | 32.96 | O |
| ATOM | 1763 | CB | VAL | A | 232 | 33.422 | 36.918 | 38.332 | 1.00 | 32.04 | C |
| ATOM | 1764 | CG1 | VAL | A | 232 | 34.131 | 35.666 | 38.721 | 1.00 | 31.82 | C |
| ATOM | 1765 | CG2 | VAL | A | 232 | 33.601 | 37.221 | 36.851 | 1.00 | 31.85 | C |
| ATOM | 1766 | N | HIS | A | 233 | 31.918 | 36.650 | 41.124 | 1.00 | 32.61 | N |
| ATOM | 1767 | CA | HIS | A | 233 | 31.819 | 35.910 | 42.376 | 1.00 | 32.41 | C |
| ATOM | 1768 | C | HIS | A | 233 | 30.383 | 35.727 | 42.874 | 1.00 | 32.27 | C |
| ATOM | 1769 | O | HIS | A | 233 | 30.134 | 35.052 | 43.860 | 1.00 | 32.05 | O |
| ATOM | 1770 | CB | HIS | A | 233 | 32.667 | 36.577 | 43.458 | 1.00 | 32.52 | C |
| ATOM | 1771 | CG | HIS | A | 233 | 34.135 | 36.579 | 43.164 | 1.00 | 33.14 | C |
| ATOM | 1772 | ND1 | HIS | A | 233 | 34.787 | 37.672 | 42.631 | 1.00 | 34.57 | N |
| ATOM | 1773 | CD2 | HIS | A | 233 | 35.083 | 35.629 | 43.342 | 1.00 | 34.15 | C |
| ATOM | 1774 | CE1 | HIS | A | 233 | 36.071 | 37.398 | 42.497 | 1.00 | 34.40 | C |
| ATOM | 1775 | NE2 | HIS | A | 233 | 36.278 | 36.164 | 42.922 | 1.00 | 35.34 | N |
| ATOM | 1776 | N | HIS | A | 234 | 29.423 | 36.314 | 42.194 | 1.00 | 32.53 | N |
| ATOM | 1777 | CA | HIS | A | 234 | 28.038 | 36.145 | 42.604 | 1.00 | 33.01 | C |
| ATOM | 1778 | C | HIS | A | 234 | 27.503 | 34.834 | 42.094 | 1.00 | 33.09 | C |
| ATOM | 1779 | O | HIS | A | 234 | 27.932 | 34.325 | 41.068 | 1.00 | 33.26 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1780 | CB | HIS | A | 234 | 27.221 | 37.276 | 42.024 | 1.00 | 33.15 | C |
| ATOM | 1781 | CG | HIS | A | 234 | 25.817 | 37.383 | 42.531 | 1.00 | 32.96 | C |
| ATOM | 1782 | ND1 | HIS | A | 234 | 24.767 | 36.704 | 41.951 | 1.00 | 32.53 | N |
| ATOM | 1783 | CD2 | HIS | A | 234 | 25.268 | 38.191 | 43.471 | 1.00 | 32.12 | C |
| ATOM | 1784 | CE1 | HIS | A | 234 | 23.639 | 37.056 | 42.540 | 1.00 | 32.45 | C |
| ATOM | 1785 | NE2 | HIS | A | 234 | 23.916 | 37.953 | 43.470 | 1.00 | 32.09 | N |
| ATOM | 1786 | N | PRO | A | 235 | 26.571 | 34.263 | 42.827 | 1.00 | 33.15 | N |
| ATOM | 1787 | CA | PRO | A | 235 | 25.985 | 32.996 | 42.410 | 1.00 | 32.79 | C |
| ATOM | 1788 | C | PRO | A | 235 | 25.386 | 33.045 | 41.026 | 1.00 | 32.62 | C |
| ATOM | 1789 | O | PRO | A | 235 | 25.210 | 31.990 | 40.440 | 1.00 | 32.65 | O |
| ATOM | 1790 | CB | PRO | A | 235 | 24.897 | 32.773 | 43.450 | 1.00 | 33.00 | C |
| ATOM | 1791 | CG | PRO | A | 235 | 25.412 | 33.500 | 44.672 | 1.00 | 32.79 | C |
| ATOM | 1792 | CD | PRO | A | 235 | 26.049 | 34.725 | 44.128 | 1.00 | 33.00 | C |
| ATOM | 1793 | N | CYS | A | 236 | 25.095 | 34.226 | 40.493 | 1.00 | 32.39 | N |
| ATOM | 1794 | CA | CYS | A | 236 | 24.487 | 34.286 | 39.185 | 1.00 | 32.11 | C |
| ATOM | 1795 | C | CYS | A | 236 | 25.529 | 34.640 | 38.139 | 1.00 | 32.34 | C |
| ATOM | 1796 | O | CYS | A | 236 | 25.217 | 35.034 | 37.018 | 1.00 | 32.23 | O |
| ATOM | 1797 | CB | CYS | A | 236 | 23.270 | 35.192 | 39.206 | 1.00 | 32.02 | C |
| ATOM | 1798 | SG | CYS | A | 236 | 21.990 | 34.545 | 40.326 | 1.00 | 32.09 | S |
| ATOM | 1799 | N | ASP | A | 237 | 26.789 | 34.456 | 38.511 | 1.00 | 32.71 | N |
| ATOM | 1800 | CA | ASP | A | 237 | 27.883 | 34.609 | 37.576 | 1.00 | 33.21 | C |
| ATOM | 1801 | C | ASP | A | 237 | 27.518 | 34.022 | 36.211 | 1.00 | 33.63 | C |
| ATOM | 1802 | O | ASP | A | 237 | 27.042 | 32.911 | 36.095 | 1.00 | 33.33 | O |
| ATOM | 1803 | CB | ASP | A | 237 | 29.139 | 33.964 | 38.132 | 1.00 | 33.01 | C |
| ATOM | 1804 | CG | ASP | A | 237 | 30.283 | 33.981 | 37.151 | 1.00 | 33.76 | C |
| ATOM | 1805 | OD1 | ASP | A | 237 | 30.340 | 34.874 | 36.279 | 1.00 | 34.52 | O |
| ATOM | 1806 | OD2 | ASP | A | 237 | 31.193 | 33.135 | 37.181 | 1.00 | 36.09 | O |
| ATOM | 1807 | N | ARG | A | 238 | 27.731 | 34.821 | 35.180 | 1.00 | 34.68 | N |
| ATOM | 1808 | CA | ARG | A | 238 | 27.414 | 34.451 | 33.810 | 1.00 | 35.15 | C |
| ATOM | 1809 | C | ARG | A | 238 | 25.962 | 34.690 | 33.375 | 1.00 | 34.98 | C |
| ATOM | 1810 | O | ARG | A | 238 | 25.664 | 34.543 | 32.197 | 1.00 | 34.26 | O |
| ATOM | 1811 | CB | ARG | A | 238 | 27.819 | 33.020 | 33.561 | 1.00 | 35.64 | C |
| ATOM | 1812 | CG | ARG | A | 238 | 29.286 | 32.847 | 33.620 | 1.00 | 36.86 | C |
| ATOM | 1813 | CD | ARG | A | 238 | 29.682 | 31.474 | 33.268 | 1.00 | 38.59 | C |
| ATOM | 1814 | NE | ARG | A | 238 | 29.321 | 30.549 | 34.338 | 1.00 | 41.64 | N |
| ATOM | 1815 | CZ | ARG | A | 238 | 28.265 | 29.755 | 34.286 | 1.00 | 43.17 | C |
| ATOM | 1816 | NH1 | ARG | A | 238 | 27.459 | 29.802 | 33.218 | 1.00 | 44.38 | N |
| ATOM | 1817 | NH2 | ARG | A | 238 | 28.006 | 28.923 | 35.291 | 1.00 | 42.18 | N |
| ATOM | 1818 | N | GLN | A | 239 | 25.067 | 35.044 | 34.303 | 1.00 | 35.13 | N |
| ATOM | 1819 | CA | GLN | A | 239 | 23.683 | 35.360 | 33.920 | 1.00 | 35.13 | C |
| ATOM | 1820 | C | GLN | A | 239 | 23.558 | 36.872 | 33.825 | 1.00 | 34.56 | C |
| ATOM | 1821 | O | GLN | A | 239 | 24.240 | 37.587 | 34.539 | 1.00 | 34.65 | O |
| ATOM | 1822 | CB | GLN | A | 239 | 22.646 | 34.839 | 34.921 | 1.00 | 35.27 | C |
| ATOM | 1823 | CG | GLN | A | 239 | 22.952 | 33.510 | 35.566 | 1.00 | 37.30 | C |
| ATOM | 1824 | CD | GLN | A | 239 | 23.270 | 32.431 | 34.552 | 1.00 | 41.59 | C |
| ATOM | 1825 | OE1 | GLN | A | 239 | 22.418 | 32.072 | 33.726 | 1.00 | 45.42 | O |
| ATOM | 1826 | NE2 | GLN | A | 239 | 24.491 | 31.899 | 34.609 | 1.00 | 42.92 | N |
| ATOM | 1827 | N | SER | A | 240 | 22.705 | 37.358 | 32.930 | 1.00 | 33.99 | N |
| ATOM | 1828 | CA | SER | A | 240 | 22.455 | 38.785 | 32.802 | 1.00 | 33.14 | C |
| ATOM | 1829 | C | SER | A | 240 | 21.613 | 39.254 | 33.957 | 1.00 | 32.53 | C |
| ATOM | 1830 | O | SER | A | 240 | 20.773 | 38.528 | 34.446 | 1.00 | 31.77 | O |
| ATOM | 1831 | CB | SER | A | 240 | 21.663 | 39.077 | 31.542 | 1.00 | 33.15 | C |
| ATOM | 1832 | OG | SER | A | 240 | 20.971 | 40.309 | 31.668 | 1.00 | 33.28 | O |
| ATOM | 1833 | N | GLN | A | 241 | 21.805 | 40.492 | 34.371 | 1.00 | 32.52 | N |
| ATOM | 1834 | CA | GLN | A | 241 | 21.022 | 41.025 | 35.476 | 1.00 | 32.54 | C |
| ATOM | 1835 | C | GLN | A | 241 | 19.711 | 41.629 | 35.001 | 1.00 | 32.44 | C |
| ATOM | 1836 | O | GLN | A | 241 | 18.872 | 42.019 | 35.804 | 1.00 | 32.16 | O |
| ATOM | 1837 | CB | GLN | A | 241 | 21.791 | 42.116 | 36.196 | 1.00 | 32.36 | C |
| ATOM | 1838 | CG | GLN | A | 241 | 22.995 | 41.669 | 36.917 | 1.00 | 32.74 | C |
| ATOM | 1839 | CD | GLN | A | 241 | 23.760 | 42.837 | 37.450 | 1.00 | 33.65 | C |
| ATOM | 1840 | OE1 | GLN | A | 241 | 23.353 | 43.442 | 38.428 | 1.00 | 34.26 | O |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1841 | NE2 | GLN | A | 241 | 24.858 | 43.182 | 36.794 | 1.00 | 35.62 | N |
| ATOM | 1842 | N | VAL | A | 242 | 19.513 | 41.708 | 33.705 | 1.00 | 32.07 | N |
| ATOM | 1843 | CA | VAL | A | 242 | 18.357 | 42.412 | 33.255 | 1.00 | 32.29 | C |
| ATOM | 1844 | C | VAL | A | 242 | 17.162 | 41.521 | 33.265 | 1.00 | 31.93 | C |
| ATOM | 1845 | O | VAL | A | 242 | 17.221 | 40.442 | 32.734 | 1.00 | 32.93 | O |
| ATOM | 1846 | CB | VAL | A | 242 | 18.516 | 42.848 | 31.808 | 1.00 | 32.63 | C |
| ATOM | 1847 | CG1 | VAL | A | 242 | 17.252 | 43.532 | 31.320 | 1.00 | 32.50 | C |
| ATOM | 1848 | CG2 | VAL | A | 242 | 19.717 | 43.714 | 31.655 | 1.00 | 33.06 | C |
| ATOM | 1849 | N | ASP | A | 243 | 16.067 | 41.977 | 33.838 | 1.00 | 31.76 | N |
| ATOM | 1850 | CA | ASP | A | 243 | 14.812 | 41.271 | 33.714 | 1.00 | 31.73 | C |
| ATOM | 1851 | C | ASP | A | 243 | 14.177 | 41.559 | 32.346 | 1.00 | 31.87 | C |
| ATOM | 1852 | O | ASP | A | 243 | 13.536 | 42.595 | 32.150 | 1.00 | 31.46 | O |
| ATOM | 1853 | CB | ASP | A | 243 | 13.861 | 41.689 | 34.830 | 1.00 | 31.61 | C |
| ATOM | 1854 | CG | ASP | A | 243 | 12.488 | 41.049 | 34.708 | 1.00 | 32.08 | C |
| ATOM | 1855 | OD1 | ASP | A | 243 | 12.164 | 40.448 | 33.655 | 1.00 | 30.69 | O |
| ATOM | 1856 | OD2 | ASP | A | 243 | 11.654 | 41.103 | 35.635 | 1.00 | 33.90 | O |
| ATOM | 1857 | N | PHE | A | 244 | 14.326 | 40.623 | 31.410 | 1.00 | 32.16 | N |
| ATOM | 1858 | CA | PHE | A | 244 | 13.746 | 40.787 | 30.075 | 1.00 | 32.29 | C |
| ATOM | 1859 | C | PHE | A | 244 | 12.252 | 41.087 | 30.092 | 1.00 | 32.74 | C |
| ATOM | 1860 | O | PHE | A | 244 | 11.741 | 41.694 | 29.162 | 1.00 | 32.51 | O |
| ATOM | 1861 | CB | PHE | A | 244 | 13.963 | 39.559 | 29.220 | 1.00 | 31.99 | C |
| ATOM | 1862 | CG | PHE | A | 244 | 15.327 | 39.446 | 28.650 | 1.00 | 31.29 | C |
| ATOM | 1863 | CD1 | PHE | A | 244 | 16.436 | 39.886 | 29.342 | 1.00 | 31.05 | C |
| ATOM | 1864 | CD2 | PHE | A | 244 | 15.500 | 38.861 | 27.421 | 1.00 | 31.04 | C |
| ATOM | 1865 | CE1 | PHE | A | 244 | 17.684 | 39.733 | 28.815 | 1.00 | 31.37 | C |
| ATOM | 1866 | CE2 | PHE | A | 244 | 16.742 | 38.709 | 26.888 | 1.00 | 31.39 | C |
| ATOM | 1867 | CZ | PHE | A | 244 | 17.839 | 39.141 | 27.584 | 1.00 | 31.77 | C |
| ATOM | 1868 | N | ASP | A | 245 | 11.547 | 40.646 | 31.124 | 1.00 | 33.52 | N |
| ATOM | 1869 | CA | ASP | A | 245 | 10.130 | 40.946 | 31.214 | 1.00 | 34.33 | C |
| ATOM | 1870 | C | ASP | A | 245 | 9.831 | 42.375 | 31.606 | 1.00 | 34.52 | C |
| ATOM | 1871 | O | ASP | A | 245 | 8.789 | 42.902 | 31.251 | 1.00 | 34.40 | O |
| ATOM | 1872 | CB | ASP | A | 245 | 9.448 | 40.015 | 32.188 | 1.00 | 34.59 | C |
| ATOM | 1873 | CG | ASP | A | 245 | 9.361 | 38.639 | 31.658 | 1.00 | 35.47 | C |
| ATOM | 1874 | OD1 | ASP | A | 245 | 9.282 | 38.519 | 30.420 | 1.00 | 36.40 | O |
| ATOM | 1875 | OD2 | ASP | A | 245 | 9.384 | 37.624 | 32.383 | 1.00 | 37.65 | O |
| ATOM | 1876 | N | ASN | A | 246 | 10.737 | 43.000 | 32.339 | 1.00 | 35.03 | N |
| ATOM | 1877 | CA | ASN | A | 246 | 10.531 | 44.364 | 32.776 | 1.00 | 35.38 | C |
| ATOM | 1878 | C | ASN | A | 246 | 11.873 | 45.003 | 32.896 | 1.00 | 34.97 | C |
| ATOM | 1879 | O | ASN | A | 246 | 12.370 | 45.160 | 33.994 | 1.00 | 35.01 | O |
| ATOM | 1880 | CB | ASN | A | 246 | 9.843 | 44.397 | 34.136 | 1.00 | 35.69 | C |
| ATOM | 1881 | CG | ASN | A | 246 | 9.395 | 45.800 | 34.533 | 1.00 | 37.41 | C |
| ATOM | 1882 | OD1 | ASN | A | 246 | 9.241 | 46.691 | 33.682 | 1.00 | 38.99 | O |
| ATOM | 1883 | ND2 | ASN | A | 246 | 9.186 | 46.006 | 35.836 | 1.00 | 38.90 | N |
| ATOM | 1884 | N | PRO | A | 247 | 12.468 | 45.357 | 31.766 | 1.00 | 34.87 | N |
| ATOM | 1885 | CA | PRO | A | 247 | 13.816 | 45.931 | 31.766 | 1.00 | 34.87 | C |
| ATOM | 1886 | C | PRO | A | 247 | 13.868 | 47.295 | 32.407 | 1.00 | 34.83 | C |
| ATOM | 1887 | O | PRO | A | 247 | 13.038 | 48.159 | 32.127 | 1.00 | 34.82 | O |
| ATOM | 1888 | CB | PRO | A | 247 | 14.184 | 46.046 | 30.288 | 1.00 | 34.75 | C |
| ATOM | 1889 | CG | PRO | A | 247 | 13.028 | 45.475 | 29.507 | 1.00 | 34.95 | C |
| ATOM | 1890 | CD | PRO | A | 247 | 11.892 | 45.241 | 30.419 | 1.00 | 34.75 | C |
| ATOM | 1891 | N | ASP | A | 248 | 14.861 | 47.448 | 33.270 | 1.00 | 34.67 | N |
| ATOM | 1892 | CA | ASP | A | 248 | 15.112 | 48.654 | 34.003 | 1.00 | 34.76 | C |
| ATOM | 1893 | C | ASP | A | 248 | 16.205 | 49.419 | 33.294 | 1.00 | 34.89 | C |
| ATOM | 1894 | O | ASP | A | 248 | 17.395 | 49.240 | 33.568 | 1.00 | 34.59 | O |
| ATOM | 1895 | CB | ASP | A | 248 | 15.583 | 48.265 | 35.387 | 1.00 | 34.87 | C |
| ATOM | 1896 | CG | ASP | A | 248 | 15.703 | 49.433 | 36.329 | 1.00 | 35.10 | C |
| ATOM | 1897 | OD1 | ASP | A | 248 | 15.958 | 50.583 | 35.902 | 1.00 | 34.24 | O |
| ATOM | 1898 | OD2 | ASP | A | 248 | 15.574 | 49.259 | 37.550 | 1.00 | 36.72 | O |
| ATOM | 1899 | N | TYR | A | 249 | 15.793 | 50.302 | 32.399 | 1.00 | 35.08 | N |
| ATOM | 1900 | CA | TYR | A | 249 | 16.743 | 51.063 | 31.615 | 1.00 | 35.24 | C |
| ATOM | 1901 | C | TYR | A | 249 | 17.578 | 52.071 | 32.400 | 1.00 | 35.48 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 1902 | O | TYR | A | 249 | 18.570 | 52.567 | 31.880 | 1.00 | 35.44 | O |
| ATOM | 1903 | CB | TYR | A | 249 | 16.021 | 51.741 | 30.465 | 1.00 | 35.05 | C |
| ATOM | 1904 | CG | TYR | A | 249 | 15.304 | 50.761 | 29.586 | 1.00 | 34.41 | C |
| ATOM | 1905 | CD1 | TYR | A | 249 | 15.977 | 49.718 | 28.971 | 1.00 | 34.17 | C |
| ATOM | 1906 | CD2 | TYR | A | 249 | 13.955 | 50.865 | 29.383 | 1.00 | 34.14 | C |
| ATOM | 1907 | CE1 | TYR | A | 249 | 15.312 | 48.828 | 28.172 | 1.00 | 33.95 | C |
| ATOM | 1908 | CE2 | TYR | A | 249 | 13.287 | 49.983 | 28.595 | 1.00 | 33.71 | C |
| ATOM | 1909 | CZ | TYR | A | 249 | 13.954 | 48.974 | 27.989 | 1.00 | 34.19 | C |
| ATOM | 1910 | OH | TYR | A | 249 | 13.232 | 48.113 | 27.194 | 1.00 | 35.64 | O |
| ATOM | 1911 | N | GLU | A | 250 | 17.207 | 52.393 | 33.631 | 1.00 | 35.82 | N |
| ATOM | 1912 | CA | GLU | A | 250 | 18.072 | 53.273 | 34.399 | 1.00 | 36.69 | C |
| ATOM | 1913 | C | GLU | A | 250 | 19.331 | 52.562 | 34.834 | 1.00 | 36.69 | C |
| ATOM | 1914 | O | GLU | A | 250 | 20.424 | 53.102 | 34.715 | 1.00 | 36.84 | O |
| ATOM | 1915 | CB | GLU | A | 250 | 17.369 | 53.836 | 35.607 | 1.00 | 37.10 | C |
| ATOM | 1916 | CG | GLU | A | 250 | 16.173 | 54.653 | 35.195 | 1.00 | 39.48 | C |
| ATOM | 1917 | CD | GLU | A | 250 | 15.559 | 55.362 | 36.359 | 1.00 | 42.67 | C |
| ATOM | 1918 | OE1 | GLU | A | 250 | 16.128 | 55.258 | 37.469 | 1.00 | 45.95 | O |
| ATOM | 1919 | OE2 | GLU | A | 250 | 14.529 | 56.030 | 36.160 | 1.00 | 44.93 | O |
| ATOM | 1920 | N | ARG | A | 251 | 19.202 | 51.344 | 35.332 | 1.00 | 36.55 | N |
| ATOM | 1921 | CA | ARG | A | 251 | 20.389 | 50.666 | 35.773 | 1.00 | 36.36 | C |
| ATOM | 1922 | C | ARG | A | 251 | 21.124 | 50.162 | 34.584 | 1.00 | 35.91 | C |
| ATOM | 1923 | O | ARG | A | 251 | 22.347 | 50.117 | 34.588 | 1.00 | 36.89 | O |
| ATOM | 1924 | CB | ARG | A | 251 | 20.062 | 49.495 | 36.697 | 1.00 | 36.66 | C |
| ATOM | 1925 | CG | ARG | A | 251 | 19.329 | 49.936 | 37.981 | 1.00 | 38.10 | C |
| ATOM | 1926 | CD | ARG | A | 251 | 18.848 | 48.824 | 38.916 | 1.00 | 39.00 | C |
| ATOM | 1927 | NE | ARG | A | 251 | 19.969 | 48.005 | 39.371 | 1.00 | 40.55 | N |
| ATOM | 1928 | CZ | ARG | A | 251 | 19.895 | 46.712 | 39.648 | 1.00 | 41.33 | C |
| ATOM | 1929 | NH1 | ARG | A | 251 | 18.742 | 46.068 | 39.542 | 1.00 | 42.58 | N |
| ATOM | 1930 | NH2 | ARG | A | 251 | 20.978 | 46.058 | 40.025 | 1.00 | 41.49 | N |
| ATOM | 1931 | N | PHE | A | 252 | 20.388 | 49.807 | 33.545 | 1.00 | 35.06 | N |
| ATOM | 1932 | CA | PHE | A | 252 | 20.988 | 49.065 | 32.455 | 1.00 | 34.37 | C |
| ATOM | 1933 | C | PHE | A | 252 | 20.653 | 49.675 | 31.138 | 1.00 | 33.82 | C |
| ATOM | 1934 | O | PHE | A | 252 | 20.048 | 49.042 | 30.278 | 1.00 | 33.57 | O |
| ATOM | 1935 | CB | PHE | A | 252 | 20.429 | 47.662 | 32.458 | 1.00 | 34.19 | C |
| ATOM | 1936 | CG | PHE | A | 252 | 20.404 | 47.019 | 33.803 | 1.00 | 33.98 | C |
| ATOM | 1937 | CD1 | PHE | A | 252 | 21.559 | 46.855 | 34.532 | 1.00 | 33.98 | C |
| ATOM | 1938 | CD2 | PHE | A | 252 | 19.220 | 46.560 | 34.337 | 1.00 | 32.84 | C |
| ATOM | 1939 | CE1 | PHE | A | 252 | 21.519 | 46.238 | 35.760 | 1.00 | 33.51 | C |
| ATOM | 1940 | CE2 | PHE | A | 252 | 19.189 | 45.953 | 35.560 | 1.00 | 32.14 | C |
| ATOM | 1941 | CZ | PHE | A | 252 | 20.327 | 45.789 | 36.269 | 1.00 | 31.96 | C |
| ATOM | 1942 | N | PRO | A | 253 | 21.087 | 50.903 | 30.959 | 1.00 | 33.27 | N |
| ATOM | 1943 | CA | PRO | A | 253 | 20.677 | 51.675 | 29.795 | 1.00 | 32.92 | C |
| ATOM | 1944 | C | PRO | A | 253 | 21.008 | 50.995 | 28.470 | 1.00 | 32.86 | C |
| ATOM | 1945 | O | PRO | A | 253 | 20.215 | 51.136 | 27.541 | 1.00 | 32.58 | O |
| ATOM | 1946 | CB | PRO | A | 253 | 21.464 | 52.957 | 29.962 | 1.00 | 32.58 | C |
| ATOM | 1947 | CG | PRO | A | 253 | 22.584 | 52.562 | 30.808 | 1.00 | 32.44 | C |
| ATOM | 1948 | CD | PRO | A | 253 | 22.038 | 51.640 | 31.802 | 1.00 | 32.67 | C |
| ATOM | 1949 | N | ASN | A | 254 | 22.108 | 50.253 | 28.359 | 1.00 | 32.60 | N |
| ATOM | 1950 | CA | ASN | A | 254 | 22.419 | 49.726 | 27.037 | 1.00 | 32.87 | C |
| ATOM | 1951 | C | ASN | A | 254 | 21.564 | 48.569 | 26.615 | 1.00 | 32.59 | C |
| ATOM | 1952 | O | ASN | A | 254 | 21.671 | 48.088 | 25.503 | 1.00 | 32.69 | O |
| ATOM | 1953 | CB | ASN | A | 254 | 23.892 | 49.414 | 26.852 | 1.00 | 32.72 | C |
| ATOM | 1954 | CG | ASN | A | 254 | 24.710 | 50.665 | 26.745 | 1.00 | 33.92 | C |
| ATOM | 1955 | OD1 | ASN | A | 254 | 25.428 | 51.022 | 27.672 | 1.00 | 37.05 | O |
| ATOM | 1956 | ND2 | ASN | A | 254 | 24.569 | 51.380 | 25.626 | 1.00 | 34.86 | N |
| ATOM | 1957 | N | PHE | A | 255 | 20.690 | 48.124 | 27.491 | 1.00 | 32.37 | N |
| ATOM | 1958 | CA | PHE | A | 255 | 19.834 | 47.057 | 27.101 | 1.00 | 32.19 | C |
| ATOM | 1959 | C | PHE | A | 255 | 18.932 | 47.578 | 26.006 | 1.00 | 32.36 | C |
| ATOM | 1960 | O | PHE | A | 255 | 18.267 | 46.819 | 25.326 | 1.00 | 32.64 | O |
| ATOM | 1961 | CB | PHE | A | 255 | 18.990 | 46.572 | 28.250 | 1.00 | 31.93 | C |
| ATOM | 1962 | CG | PHE | A | 255 | 18.249 | 45.354 | 27.918 | 1.00 | 31.43 | C |

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ATOM   1963  CD1 PHE A 255      18.919  44.176  27.718  1.00 33.75           C
ATOM   1964  CD2 PHE A 255      16.909  45.392  27.718  1.00 31.23           C
ATOM   1965  CE1 PHE A 255      18.239  43.035  27.367  1.00 34.05           C
ATOM   1966  CE2 PHE A 255      16.230  44.275  27.380  1.00 32.00           C
ATOM   1967  CZ  PHE A 255      16.890  43.088  27.203  1.00 32.84           C
ATOM   1968  N   GLN A 256      18.890  48.888  25.844  1.00 32.46           N
ATOM   1969  CA  GLN A 256      18.078  49.456  24.794  1.00 32.37           C
ATOM   1970  C   GLN A 256      18.776  49.342  23.455  1.00 32.34           C
ATOM   1971  O   GLN A 256      18.260  49.815  22.470  1.00 32.11           O
ATOM   1972  CB  GLN A 256      17.777  50.924  25.061  1.00 32.28           C
ATOM   1973  CG  GLN A 256      16.775  51.169  26.144  1.00 32.39           C
ATOM   1974  CD  GLN A 256      16.823  52.594  26.645  1.00 32.91           C
ATOM   1975  OE1 GLN A 256      15.830  53.303  26.588  1.00 34.66           O
ATOM   1976  NE2 GLN A 256      17.982  53.021  27.125  1.00 32.30           N
ATOM   1977  N   ASN A 257      19.956  48.744  23.404  1.00 32.78           N
ATOM   1978  CA  ASN A 257      20.634  48.617  22.126  1.00 33.17           C
ATOM   1979  C   ASN A 257      20.828  47.159  21.763  1.00 34.01           C
ATOM   1980  O   ASN A 257      21.406  46.841  20.721  1.00 34.41           O
ATOM   1981  CB  ASN A 257      21.998  49.310  22.140  1.00 32.88           C
ATOM   1982  CG  ASN A 257      21.928  50.750  22.595  1.00 31.31           C
ATOM   1983  OD1 ASN A 257      22.471  51.105  23.639  1.00 27.26           O
ATOM   1984  ND2 ASN A 257      21.283  51.595  21.797  1.00 29.34           N
ATOM   1985  N   VAL A 258      20.338  46.263  22.606  1.00 34.66           N
ATOM   1986  CA  VAL A 258      20.565  44.855  22.370  1.00 35.33           C
ATOM   1987  C   VAL A 258      19.832  44.361  21.130  1.00 35.37           C
ATOM   1988  O   VAL A 258      18.751  44.832  20.813  1.00 34.96           O
ATOM   1989  CB  VAL A 258      20.144  44.010  23.558  1.00 35.59           C
ATOM   1990  CG1 VAL A 258      18.632  43.851  23.604  1.00 35.73           C
ATOM   1991  CG2 VAL A 258      20.780  42.662  23.428  1.00 36.60           C
ATOM   1992  N   VAL A 259      20.447  43.418  20.428  1.00 35.87           N
ATOM   1993  CA  VAL A 259      19.853  42.844  19.230  1.00 36.40           C
ATOM   1994  C   VAL A 259      20.125  41.355  19.148  1.00 36.66           C
ATOM   1995  O   VAL A 259      21.282  40.943  19.102  1.00 36.47           O
ATOM   1996  CB  VAL A 259      20.450  43.459  17.969  1.00 36.47           C
ATOM   1997  CG1 VAL A 259      19.830  42.822  16.764  1.00 36.75           C
ATOM   1998  CG2 VAL A 259      20.212  44.931  17.932  1.00 36.66           C
ATOM   1999  N   GLY A 260      19.066  40.551  19.085  1.00 37.15           N
ATOM   2000  CA  GLY A 260      19.215  39.096  19.067  1.00 37.50           C
ATOM   2001  C   GLY A 260      19.132  38.328  17.745  1.00 37.55           C
ATOM   2002  O   GLY A 260      18.716  38.839  16.704  1.00 37.45           O
ATOM   2003  N   TYR A 261      19.578  37.079  17.817  1.00 37.54           N
ATOM   2004  CA  TYR A 261      19.466  36.113  16.744  1.00 37.52           C
ATOM   2005  C   TYR A 261      18.530  35.107  17.358  1.00 37.09           C
ATOM   2006  O   TYR A 261      18.788  34.648  18.466  1.00 37.12           O
ATOM   2007  CB  TYR A 261      20.796  35.429  16.481  1.00 37.79           C
ATOM   2008  CG  TYR A 261      21.838  36.327  15.874  1.00 39.43           C
ATOM   2009  CD1 TYR A 261      22.005  36.380  14.507  1.00 41.03           C
ATOM   2010  CD2 TYR A 261      22.648  37.125  16.662  1.00 41.07           C
ATOM   2011  CE1 TYR A 261      22.937  37.193  13.940  1.00 41.71           C
ATOM   2012  CE2 TYR A 261      23.593  37.938  16.093  1.00 41.99           C
ATOM   2013  CZ  TYR A 261      23.725  37.960  14.728  1.00 42.45           C
ATOM   2014  OH  TYR A 261      24.650  38.762  14.121  1.00 46.29           O
ATOM   2015  N   GLU A 262      17.430  34.773  16.699  1.00 36.56           N
ATOM   2016  CA  GLU A 262      16.500  33.866  17.346  1.00 35.87           C
ATOM   2017  C   GLU A 262      16.064  32.737  16.447  1.00 35.41           C
ATOM   2018  O   GLU A 262      16.310  32.747  15.248  1.00 35.03           O
ATOM   2019  CB  GLU A 262      15.320  34.639  17.943  1.00 35.67           C
ATOM   2020  CG  GLU A 262      14.085  34.789  17.098  1.00 35.22           C
ATOM   2021  CD  GLU A 262      13.039  35.601  17.821  1.00 35.62           C
ATOM   2022  OE1 GLU A 262      13.201  36.833  17.866  1.00 38.15           O
ATOM   2023  OE2 GLU A 262      12.074  35.031  18.367  1.00 35.12           O
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ATOM   2024  N   THR A 263      15.440  31.744  17.060  1.00 35.07           N
ATOM   2025  CA  THR A 263      15.004  30.565  16.351  1.00 34.84           C
ATOM   2026  C   THR A 263      14.138  29.670  17.224  1.00 34.38           C
ATOM   2027  O   THR A 263      14.152  29.745  18.452  1.00 34.07           O
ATOM   2028  CB  THR A 263      16.235  29.767  15.847  1.00 34.75           C
ATOM   2029  OG1 THR A 263      15.864  28.964  14.731  1.00 35.81           O
ATOM   2030  CG2 THR A 263      16.693  28.745  16.837  1.00 34.59           C
ATOM   2031  N   VAL A 264      13.368  28.820  16.573  1.00 34.02           N
ATOM   2032  CA  VAL A 264      12.597  27.854  17.306  1.00 33.95           C
ATOM   2033  C   VAL A 264      13.054  26.460  16.918  1.00 33.60           C
ATOM   2034  O   VAL A 264      12.957  26.065  15.762  1.00 33.27           O
ATOM   2035  CB  VAL A 264      11.112  28.019  17.075  1.00 33.95           C
ATOM   2036  CG1 VAL A 264      10.393  26.788  17.568  1.00 34.24           C
ATOM   2037  CG2 VAL A 264      10.615  29.247  17.823  1.00 33.85           C
ATOM   2038  N   VAL A 265      13.572  25.708  17.880  1.00 33.43           N
ATOM   2039  CA  VAL A 265      13.984  24.354  17.546  1.00 33.48           C
ATOM   2040  C   VAL A 265      12.949  23.321  17.907  1.00 32.85           C
ATOM   2041  O   VAL A 265      12.234  23.441  18.884  1.00 32.91           O
ATOM   2042  CB  VAL A 265      15.332  23.954  18.139  1.00 33.61           C
ATOM   2043  CG1 VAL A 265      16.408  24.721  17.432  1.00 34.56           C
ATOM   2044  CG2 VAL A 265      15.381  24.153  19.636  1.00 33.15           C
ATOM   2045  N   GLY A 266      12.848  22.321  17.064  1.00 32.32           N
ATOM   2046  CA  GLY A 266      11.938  21.240  17.331  1.00 32.27           C
ATOM   2047  C   GLY A 266      12.634  19.905  17.310  1.00 31.78           C
ATOM   2048  O   GLY A 266      13.852  19.799  17.124  1.00 31.15           O
ATOM   2049  N   PRO A 267      11.827  18.872  17.454  1.00 31.56           N
ATOM   2050  CA  PRO A 267      12.343  17.516  17.547  1.00 31.40           C
ATOM   2051  C   PRO A 267      13.203  17.314  16.336  1.00 31.22           C
ATOM   2052  O   PRO A 267      12.755  17.631  15.241  1.00 31.24           O
ATOM   2053  CB  PRO A 267      11.074  16.664  17.552  1.00 30.81           C
ATOM   2054  CG  PRO A 267      10.048  17.568  18.087  1.00 31.26           C
ATOM   2055  CD  PRO A 267      10.358  18.900  17.451  1.00 31.85           C
ATOM   2056  N   GLY A 268      14.445  16.891  16.536  1.00 31.06           N
ATOM   2057  CA  GLY A 268      15.334  16.620  15.426  1.00 31.07           C
ATOM   2058  C   GLY A 268      16.337  17.703  15.112  1.00 31.31           C
ATOM   2059  O   GLY A 268      17.352  17.425  14.493  1.00 31.12           O
ATOM   2060  N   ASP A 269      16.061  18.939  15.517  1.00 31.87           N
ATOM   2061  CA  ASP A 269      16.975  20.032  15.253  1.00 32.18           C
ATOM   2062  C   ASP A 269      18.117  20.099  16.282  1.00 32.69           C
ATOM   2063  O   ASP A 269      17.974  19.720  17.450  1.00 32.69           O
ATOM   2064  CB  ASP A 269      16.282  21.381  15.390  1.00 32.73           C
ATOM   2065  CG  ASP A 269      15.094  21.583  14.478  1.00 32.07           C
ATOM   2066  OD1 ASP A 269      15.023  21.039  13.367  1.00 33.96           O
ATOM   2067  OD2 ASP A 269      14.191  22.368  14.806  1.00 30.81           O
ATOM   2068  N   VAL A 270      19.234  20.667  15.854  1.00 32.97           N
ATOM   2069  CA  VAL A 270      20.376  20.839  16.715  1.00 32.97           C
ATOM   2070  C   VAL A 270      20.844  22.258  16.579  1.00 32.97           C
ATOM   2071  O   VAL A 270      21.130  22.716  15.488  1.00 33.40           O
ATOM   2072  CB  VAL A 270      21.485  19.896  16.323  1.00 32.94           C
ATOM   2073  CG1 VAL A 270      22.755  20.207  17.066  1.00 33.16           C
ATOM   2074  CG2 VAL A 270      21.069  18.519  16.646  1.00 33.14           C
ATOM   2075  N   LEU A 271      20.883  22.965  17.692  1.00 32.91           N
ATOM   2076  CA  LEU A 271      21.321  24.337  17.690  1.00 32.91           C
ATOM   2077  C   LEU A 271      22.770  24.395  18.129  1.00 32.95           C
ATOM   2078  O   LEU A 271      23.116  23.864  19.161  1.00 32.76           O
ATOM   2079  CB  LEU A 271      20.468  25.159  18.656  1.00 32.64           C
ATOM   2080  CG  LEU A 271      20.896  26.616  18.773  1.00 32.61           C
ATOM   2081  CD1 LEU A 271      20.989  27.276  17.405  1.00 32.23           C
ATOM   2082  CD2 LEU A 271      19.936  27.383  19.638  1.00 33.12           C
ATOM   2083  N   TYR A 272      23.633  25.006  17.333  1.00 33.19           N
ATOM   2084  CA  TYR A 272      24.989  25.215  17.791  1.00 33.39           C
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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2085 | C | TYR | A | 272 | 25.004 | 26.517 | 18.554 | 1.00 | 33.40 | C |
| ATOM | 2086 | O | TYR | A | 272 | 24.834 | 27.560 | 17.950 | 1.00 | 33.42 | O |
| ATOM | 2087 | CB | TYR | A | 272 | 25.991 | 25.297 | 16.633 | 1.00 | 33.28 | C |
| ATOM | 2088 | CG | TYR | A | 272 | 27.376 | 25.802 | 17.039 | 1.00 | 32.43 | C |
| ATOM | 2089 | CD1 | TYR | A | 272 | 28.005 | 25.340 | 18.179 | 1.00 | 31.06 | C |
| ATOM | 2090 | CD2 | TYR | A | 272 | 28.047 | 26.746 | 16.267 | 1.00 | 32.28 | C |
| ATOM | 2091 | CE1 | TYR | A | 272 | 29.265 | 25.805 | 18.544 | 1.00 | 30.52 | C |
| ATOM | 2092 | CE2 | TYR | A | 272 | 29.300 | 27.213 | 16.622 | 1.00 | 30.88 | C |
| ATOM | 2093 | CZ | TYR | A | 272 | 29.906 | 26.737 | 17.759 | 1.00 | 29.92 | C |
| ATOM | 2094 | OH | TYR | A | 272 | 31.146 | 27.216 | 18.113 | 1.00 | 27.15 | O |
| ATOM | 2095 | N | ILE | A | 273 | 25.178 | 26.438 | 19.872 | 1.00 | 33.69 | N |
| ATOM | 2096 | CA | ILE | A | 273 | 25.350 | 27.609 | 20.734 | 1.00 | 33.97 | C |
| ATOM | 2097 | C | ILE | A | 273 | 26.830 | 27.759 | 21.068 | 1.00 | 34.43 | C |
| ATOM | 2098 | O | ILE | A | 273 | 27.332 | 27.113 | 21.998 | 1.00 | 34.76 | O |
| ATOM | 2099 | CB | ILE | A | 273 | 24.595 | 27.436 | 22.032 | 1.00 | 33.75 | C |
| ATOM | 2100 | CG1 | ILE | A | 273 | 23.122 | 27.219 | 21.749 | 1.00 | 33.59 | C |
| ATOM | 2101 | CG2 | ILE | A | 273 | 24.779 | 28.654 | 22.896 | 1.00 | 33.60 | C |
| ATOM | 2102 | CD1 | ILE | A | 273 | 22.306 | 26.986 | 22.984 | 1.00 | 33.23 | C |
| ATOM | 2103 | N | PRO | A | 274 | 27.519 | 28.630 | 20.345 | 1.00 | 34.61 | N |
| ATOM | 2104 | CA | PRO | A | 274 | 28.965 | 28.780 | 20.485 | 1.00 | 34.92 | C |
| ATOM | 2105 | C | PRO | A | 274 | 29.348 | 29.378 | 21.803 | 1.00 | 35.17 | C |
| ATOM | 2106 | O | PRO | A | 274 | 28.639 | 30.252 | 22.300 | 1.00 | 35.16 | O |
| ATOM | 2107 | CB | PRO | A | 274 | 29.333 | 29.771 | 19.382 | 1.00 | 35.09 | C |
| ATOM | 2108 | CG | PRO | A | 274 | 28.113 | 29.929 | 18.551 | 1.00 | 35.02 | C |
| ATOM | 2109 | CD | PRO | A | 274 | 26.957 | 29.584 | 19.388 | 1.00 | 34.69 | C |
| ATOM | 2110 | N | MET | A | 275 | 30.476 | 28.927 | 22.339 | 1.00 | 35.69 | N |
| ATOM | 2111 | CA | MET | A | 275 | 30.982 | 29.399 | 23.622 | 1.00 | 36.15 | C |
| ATOM | 2112 | C | MET | A | 275 | 30.981 | 30.917 | 23.754 | 1.00 | 36.09 | C |
| ATOM | 2113 | O | MET | A | 275 | 31.316 | 31.635 | 22.805 | 1.00 | 36.23 | O |
| ATOM | 2114 | CB | MET | A | 275 | 32.400 | 28.928 | 23.805 | 1.00 | 36.23 | C |
| ATOM | 2115 | CG | MET | A | 275 | 32.813 | 28.928 | 25.229 | 1.00 | 38.02 | C |
| ATOM | 2116 | SD | MET | A | 275 | 34.361 | 28.108 | 25.442 | 1.00 | 42.07 | S |
| ATOM | 2117 | CE | MET | A | 275 | 35.330 | 28.680 | 23.895 | 1.00 | 42.34 | C |
| ATOM | 2118 | N | TYR | A | 276 | 30.611 | 31.401 | 24.935 | 1.00 | 35.76 | N |
| ATOM | 2119 | CA | TYR | A | 276 | 30.574 | 32.833 | 25.191 | 1.00 | 35.62 | C |
| ATOM | 2120 | C | TYR | A | 276 | 29.339 | 33.513 | 24.555 | 1.00 | 35.32 | C |
| ATOM | 2121 | O | TYR | A | 276 | 29.048 | 34.653 | 24.866 | 1.00 | 35.15 | O |
| ATOM | 2122 | CB | TYR | A | 276 | 31.921 | 33.510 | 24.804 | 1.00 | 35.75 | C |
| ATOM | 2123 | CG | TYR | A | 276 | 33.049 | 33.221 | 25.822 | 1.00 | 35.70 | C |
| ATOM | 2124 | CD1 | TYR | A | 276 | 33.036 | 33.805 | 27.077 | 1.00 | 34.51 | C |
| ATOM | 2125 | CD2 | TYR | A | 276 | 34.103 | 32.356 | 25.521 | 1.00 | 35.30 | C |
| ATOM | 2126 | CE1 | TYR | A | 276 | 34.013 | 33.549 | 27.997 | 1.00 | 34.63 | C |
| ATOM | 2127 | CE2 | TYR | A | 276 | 35.100 | 32.085 | 26.446 | 1.00 | 35.01 | C |
| ATOM | 2128 | CZ | TYR | A | 276 | 35.055 | 32.685 | 27.695 | 1.00 | 35.73 | C |
| ATOM | 2129 | OH | TYR | A | 276 | 36.051 | 32.433 | 28.657 | 1.00 | 34.27 | O |
| ATOM | 2130 | N | TRP | A | 277 | 28.573 | 32.838 | 23.708 | 1.00 | 35.19 | N |
| ATOM | 2131 | CA | TRP | A | 277 | 27.353 | 33.491 | 23.224 | 1.00 | 35.20 | C |
| ATOM | 2132 | C | TRP | A | 277 | 26.245 | 33.424 | 24.245 | 1.00 | 35.16 | C |
| ATOM | 2133 | O | TRP | A | 277 | 25.947 | 32.369 | 24.797 | 1.00 | 35.08 | O |
| ATOM | 2134 | CB | TRP | A | 277 | 26.806 | 32.880 | 21.944 | 1.00 | 35.27 | C |
| ATOM | 2135 | CG | TRP | A | 277 | 27.538 | 33.286 | 20.784 | 1.00 | 34.70 | C |
| ATOM | 2136 | CD1 | TRP | A | 277 | 28.858 | 33.128 | 20.579 | 1.00 | 35.11 | C |
| ATOM | 2137 | CD2 | TRP | A | 277 | 27.020 | 33.945 | 19.639 | 1.00 | 35.27 | C |
| ATOM | 2138 | NE1 | TRP | A | 277 | 29.213 | 33.648 | 19.361 | 1.00 | 35.58 | N |
| ATOM | 2139 | CE2 | TRP | A | 277 | 28.094 | 34.156 | 18.761 | 1.00 | 34.89 | C |
| ATOM | 2140 | CE3 | TRP | A | 277 | 25.751 | 34.388 | 19.258 | 1.00 | 35.56 | C |
| ATOM | 2141 | CZ2 | TRP | A | 277 | 27.946 | 34.781 | 17.543 | 1.00 | 32.83 | C |
| ATOM | 2142 | CZ3 | TRP | A | 277 | 25.612 | 35.012 | 18.041 | 1.00 | 34.41 | C |
| ATOM | 2143 | CH2 | TRP | A | 277 | 26.704 | 35.199 | 17.201 | 1.00 | 33.11 | C |
| ATOM | 2144 | N | TRP | A | 278 | 25.597 | 34.555 | 24.457 | 1.00 | 35.11 | N |
| ATOM | 2145 | CA | TRP | A | 278 | 24.501 | 34.612 | 25.388 | 1.00 | 35.03 | C |

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ATOM   2146  C   TRP A 278      23.334  33.859  24.838  1.00 35.14           C
ATOM   2147  O   TRP A 278      23.068  33.939  23.637  1.00 35.16           O
ATOM   2148  CB  TRP A 278      24.047  36.030  25.553  1.00 34.94           C
ATOM   2149  CG  TRP A 278      25.025  36.909  26.185  1.00 35.52           C
ATOM   2150  CD1 TRP A 278      26.030  37.597  25.584  1.00 35.77           C
ATOM   2151  CD2 TRP A 278      25.071  37.244  27.560  1.00 36.19           C
ATOM   2152  NE1 TRP A 278      26.713  38.336  26.518  1.00 36.09           N
ATOM   2153  CE2 TRP A 278      26.133  38.132  27.741  1.00 36.37           C
ATOM   2154  CE3 TRP A 278      24.312  36.876  28.668  1.00 36.48           C
ATOM   2155  CZ2 TRP A 278      26.463  38.637  28.976  1.00 37.12           C
ATOM   2156  CZ3 TRP A 278      24.636  37.375  29.877  1.00 36.37           C
ATOM   2157  CH2 TRP A 278      25.701  38.246  30.032  1.00 36.92           C
ATOM   2158  N   HIS A 279      22.620  33.133  25.692  1.00 35.10           N
ATOM   2159  CA  HIS A 279      21.400  32.516  25.218  1.00 35.20           C
ATOM   2160  C   HIS A 279      20.300  32.555  26.231  1.00 34.69           C
ATOM   2161  O   HIS A 279      20.540  32.348  27.414  1.00 34.75           O
ATOM   2162  CB  HIS A 279      21.624  31.079  24.764  1.00 35.73           C
ATOM   2163  CG  HIS A 279      22.403  30.236  25.727  1.00 37.15           C
ATOM   2164  ND1 HIS A 279      23.775  30.295  25.819  1.00 39.54           N
ATOM   2165  CD2 HIS A 279      22.010  29.283  26.609  1.00 38.10           C
ATOM   2166  CE1 HIS A 279      24.194  29.425  26.726  1.00 39.33           C
ATOM   2167  NE2 HIS A 279      23.143  28.797  27.221  1.00 37.68           N
ATOM   2168  N   HIS A 280      19.092  32.795  25.721  1.00 34.17           N
ATOM   2169  CA  HIS A 280      17.850  32.854  26.483  1.00 33.72           C
ATOM   2170  C   HIS A 280      16.960  31.779  25.901  1.00 33.50           C
ATOM   2171  O   HIS A 280      16.730  31.765  24.705  1.00 33.21           O
ATOM   2172  CB  HIS A 280      17.215  34.208  26.257  1.00 33.58           C
ATOM   2173  CG  HIS A 280      15.733  34.247  26.468  1.00 33.92           C
ATOM   2174  ND1 HIS A 280      15.151  34.997  27.464  1.00 33.67           N
ATOM   2175  CD2 HIS A 280      14.711  33.680  25.779  1.00 34.05           C
ATOM   2176  CE1 HIS A 280      13.838  34.874  27.395  1.00 33.47           C
ATOM   2177  NE2 HIS A 280      13.545  34.078  26.384  1.00 33.19           N
ATOM   2178  N   ILE A 281      16.425  30.892  26.723  1.00 33.62           N
ATOM   2179  CA  ILE A 281      15.699  29.755  26.176  1.00 33.56           C
ATOM   2180  C   ILE A 281      14.358  29.554  26.806  1.00 33.01           C
ATOM   2181  O   ILE A 281      14.242  29.475  28.012  1.00 32.55           O
ATOM   2182  CB  ILE A 281      16.554  28.501  26.300  1.00 33.91           C
ATOM   2183  CG1 ILE A 281      17.699  28.600  25.295  1.00 35.00           C
ATOM   2184  CG2 ILE A 281      15.752  27.277  25.988  1.00 34.05           C
ATOM   2185  CD1 ILE A 281      18.797  27.663  25.562  1.00 36.33           C
ATOM   2186  N   GLU A 282      13.343  29.445  25.960  1.00 33.12           N
ATOM   2187  CA  GLU A 282      11.977  29.342  26.441  1.00 33.13           C
ATOM   2188  C   GLU A 282      11.168  28.219  25.777  1.00 32.96           C
ATOM   2189  O   GLU A 282      11.252  27.988  24.577  1.00 32.94           O
ATOM   2190  CB  GLU A 282      11.290  30.707  26.327  1.00 33.06           C
ATOM   2191  CG  GLU A 282      11.065  31.250  24.925  1.00 33.43           C
ATOM   2192  CD  GLU A 282      10.529  32.682  24.951  1.00 33.96           C
ATOM   2193  OE1 GLU A 282      11.071  33.500  25.703  1.00 34.61           O
ATOM   2194  OE2 GLU A 282       9.563  33.009  24.236  1.00 35.15           O
ATOM   2195  N   SER A 283      10.431  27.497  26.607  1.00 32.96           N
ATOM   2196  CA  SER A 283       9.571  26.420  26.169  1.00 33.51           C
ATOM   2197  C   SER A 283       8.247  27.070  25.784  1.00 34.03           C
ATOM   2198  O   SER A 283       7.654  27.772  26.597  1.00 34.19           O
ATOM   2199  CB  SER A 283       9.375  25.408  27.303  1.00 33.43           C
ATOM   2200  OG  SER A 283      10.371  24.393  27.280  1.00 32.99           O
ATOM   2201  N   LEU A 284       7.769  26.828  24.565  1.00 34.36           N
ATOM   2202  CA  LEU A 284       6.610  27.553  24.081  1.00 34.81           C
ATOM   2203  C   LEU A 284       5.399  27.454  24.982  1.00 35.14           C
ATOM   2204  O   LEU A 284       5.128  26.425  25.599  1.00 35.08           O
ATOM   2205  CB  LEU A 284       6.226  27.131  22.670  1.00 35.02           C
ATOM   2206  CG  LEU A 284       7.302  27.255  21.596  1.00 35.52           C
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ATOM   2207  CD1 LEU A 284       6.675  27.427  20.231  1.00 36.06           C
ATOM   2208  CD2 LEU A 284       8.197  28.404  21.862  1.00 36.37           C
ATOM   2209  N   LEU A 285       4.674  28.561  25.040  1.00 35.48           N
ATOM   2210  CA  LEU A 285       3.481  28.641  25.832  1.00 35.85           C
ATOM   2211  C   LEU A 285       2.509  27.670  25.255  1.00 36.11           C
ATOM   2212  O   LEU A 285       2.314  27.623  24.041  1.00 36.34           O
ATOM   2213  CB  LEU A 285       2.876  30.024  25.742  1.00 35.90           C
ATOM   2214  CG  LEU A 285       3.740  31.116  26.343  1.00 36.22           C
ATOM   2215  CD1 LEU A 285       3.271  32.449  25.821  1.00 36.13           C
ATOM   2216  CD2 LEU A 285       3.701  31.034  27.861  1.00 36.27           C
ATOM   2217  N   ASN A 286       1.909  26.879  26.128  1.00 36.14           N
ATOM   2218  CA  ASN A 286       0.890  25.958  25.703  1.00 36.04           C
ATOM   2219  C   ASN A 286       1.373  24.932  24.663  1.00 35.65           C
ATOM   2220  O   ASN A 286       0.593  24.471  23.833  1.00 35.84           O
ATOM   2221  CB  ASN A 286      -0.283  26.792  25.191  1.00 36.33           C
ATOM   2222  CG  ASN A 286      -0.805  27.766  26.254  1.00 36.97           C
ATOM   2223  OD1 ASN A 286      -1.266  27.346  27.316  1.00 37.84           O
ATOM   2224  ND2 ASN A 286      -0.716  29.067  25.977  1.00 37.29           N
ATOM   2225  N   GLY A 287       2.648  24.550  24.736  1.00 35.18           N
ATOM   2226  CA  GLY A 287       3.220  23.588  23.806  1.00 34.71           C
ATOM   2227  C   GLY A 287       3.556  22.252  24.428  1.00 34.44           C
ATOM   2228  O   GLY A 287       4.071  21.349  23.764  1.00 34.53           O
ATOM   2229  N   GLY A 288       3.255  22.106  25.706  1.00 34.18           N
ATOM   2230  CA  GLY A 288       3.521  20.858  26.371  1.00 34.22           C
ATOM   2231  C   GLY A 288       4.964  20.793  26.766  1.00 34.25           C
ATOM   2232  O   GLY A 288       5.727  21.719  26.523  1.00 34.28           O
ATOM   2233  N   ILE A 289       5.351  19.674  27.349  1.00 34.55           N
ATOM   2234  CA  ILE A 289       6.671  19.572  27.918  1.00 34.83           C
ATOM   2235  C   ILE A 289       7.702  19.529  26.837  1.00 34.87           C
ATOM   2236  O   ILE A 289       7.417  19.196  25.687  1.00 35.21           O
ATOM   2237  CB  ILE A 289       6.815  18.325  28.786  1.00 35.01           C
ATOM   2238  CG1 ILE A 289       7.018  17.091  27.924  1.00 35.30           C
ATOM   2239  CG2 ILE A 289       5.610  18.143  29.694  1.00 35.22           C
ATOM   2240  CD1 ILE A 289       7.654  15.972  28.698  1.00 35.70           C
ATOM   2241  N   THR A 290       8.921  19.853  27.219  1.00 34.80           N
ATOM   2242  CA  THR A 290      10.001  19.849  26.273  1.00 34.64           C
ATOM   2243  C   THR A 290      11.103  18.951  26.740  1.00 34.30           C
ATOM   2244  O   THR A 290      11.286  18.742  27.924  1.00 34.66           O
ATOM   2245  CB  THR A 290      10.522  21.258  26.094  1.00 34.75           C
ATOM   2246  OG1 THR A 290      10.747  21.863  27.375  1.00 34.33           O
ATOM   2247  CG2 THR A 290       9.455  22.105  25.458  1.00 34.98           C
ATOM   2248  N   ILE A 291      11.832  18.395  25.802  1.00 33.95           N
ATOM   2249  CA  ILE A 291      12.940  17.576  26.176  1.00 34.07           C
ATOM   2250  C   ILE A 291      14.091  17.963  25.310  1.00 33.73           C
ATOM   2251  O   ILE A 291      13.933  18.203  24.125  1.00 33.83           O
ATOM   2252  CB  ILE A 291      12.590  16.111  26.029  1.00 34.23           C
ATOM   2253  CG1 ILE A 291      11.439  15.793  26.967  1.00 34.84           C
ATOM   2254  CG2 ILE A 291      13.758  15.248  26.429  1.00 34.60           C
ATOM   2255  CD1 ILE A 291      11.021  14.384  26.946  1.00 35.22           C
ATOM   2256  N   THR A 292      15.254  18.062  25.913  1.00 33.47           N
ATOM   2257  CA  THR A 292      16.410  18.418  25.158  1.00 33.68           C
ATOM   2258  C   THR A 292      17.579  17.741  25.748  1.00 33.73           C
ATOM   2259  O   THR A 292      17.623  17.472  26.942  1.00 33.28           O
ATOM   2260  CB  THR A 292      16.725  19.921  25.265  1.00 33.93           C
ATOM   2261  OG1 THR A 292      15.590  20.725  24.921  1.00 33.80           O
ATOM   2262  CG2 THR A 292      17.774  20.293  24.245  1.00 34.05           C
ATOM   2263  N   VAL A 293      18.565  17.518  24.906  1.00 34.13           N
ATOM   2264  CA  VAL A 293      19.821  17.030  25.391  1.00 34.56           C
ATOM   2265  C   VAL A 293      20.935  17.867  24.813  1.00 34.79           C
ATOM   2266  O   VAL A 293      21.039  18.017  23.600  1.00 34.88           O
ATOM   2267  CB  VAL A 293      20.029  15.603  25.019  1.00 34.66           C
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ATOM   2268  CG1 VAL A 293      21.473  15.238  25.222  1.00 35.24           C
ATOM   2269  CG2 VAL A 293      19.141  14.741  25.880  1.00 35.15           C
ATOM   2270  N   ASN A 294      21.768  18.433  25.681  1.00 34.82           N
ATOM   2271  CA  ASN A 294      22.890  19.187  25.174  1.00 34.61           C
ATOM   2272  C   ASN A 294      24.159  18.372  25.251  1.00 34.68           C
ATOM   2273  O   ASN A 294      24.220  17.350  25.934  1.00 34.28           O
ATOM   2274  CB  ASN A 294      23.036  20.571  25.829  1.00 34.77           C
ATOM   2275  CG  ASN A 294      23.676  20.533  27.197  1.00 33.90           C
ATOM   2276  OD1 ASN A 294      24.170  19.504  27.653  1.00 36.35           O
ATOM   2277  ND2 ASN A 294      23.658  21.670  27.868  1.00 30.46           N
ATOM   2278  N   PHE A 295      25.141  18.870  24.510  1.00 34.93           N
ATOM   2279  CA  PHE A 295      26.450  18.291  24.326  1.00 35.27           C
ATOM   2280  C   PHE A 295      27.467  19.411  24.552  1.00 35.69           C
ATOM   2281  O   PHE A 295      27.610  20.288  23.698  1.00 35.68           O
ATOM   2282  CB  PHE A 295      26.581  17.832  22.875  1.00 35.33           C
ATOM   2283  CG  PHE A 295      25.858  16.554  22.545  1.00 34.85           C
ATOM   2284  CD1 PHE A 295      24.492  16.549  22.332  1.00 35.36           C
ATOM   2285  CD2 PHE A 295      26.559  15.371  22.383  1.00 33.46           C
ATOM   2286  CE1 PHE A 295      23.841  15.378  21.996  1.00 35.19           C
ATOM   2287  CE2 PHE A 295      25.918  14.207  22.048  1.00 33.20           C
ATOM   2288  CZ  PHE A 295      24.566  14.202  21.853  1.00 34.09           C
ATOM   2289  N   TRP A 296      28.182  19.369  25.677  1.00 36.18           N
ATOM   2290  CA  TRP A 296      29.113  20.433  26.073  1.00 36.34           C
ATOM   2291  C   TRP A 296      30.534  19.963  25.938  1.00 36.50           C
ATOM   2292  O   TRP A 296      30.932  18.969  26.563  1.00 36.32           O
ATOM   2293  CB  TRP A 296      28.913  20.830  27.541  1.00 36.57           C
ATOM   2294  CG  TRP A 296      27.934  21.912  27.776  1.00 37.38           C
ATOM   2295  CD1 TRP A 296      26.997  22.361  26.909  1.00 38.36           C
ATOM   2296  CD2 TRP A 296      27.787  22.693  28.965  1.00 39.42           C
ATOM   2297  NE1 TRP A 296      26.275  23.384  27.473  1.00 38.20           N
ATOM   2298  CE2 TRP A 296      26.737  23.605  28.736  1.00 38.86           C
ATOM   2299  CE3 TRP A 296      28.450  22.730  30.204  1.00 40.74           C
ATOM   2300  CZ2 TRP A 296      26.327  24.529  29.682  1.00 41.03           C
ATOM   2301  CZ3 TRP A 296      28.037  23.665  31.160  1.00 40.86           C
ATOM   2302  CH2 TRP A 296      26.989  24.544  30.891  1.00 41.52           C
ATOM   2303  N   TYR A 297      31.303  20.719  25.162  1.00 36.60           N
ATOM   2304  CA  TYR A 297      32.703  20.442  24.923  1.00 36.79           C
ATOM   2305  C   TYR A 297      33.534  21.597  25.457  1.00 36.96           C
ATOM   2306  O   TYR A 297      33.117  22.734  25.363  1.00 36.32           O
ATOM   2307  CB  TYR A 297      32.923  20.291  23.423  1.00 36.93           C
ATOM   2308  CG  TYR A 297      32.280  19.054  22.868  1.00 37.30           C
ATOM   2309  CD1 TYR A 297      30.939  19.046  22.523  1.00 37.28           C
ATOM   2310  CD2 TYR A 297      33.008  17.880  22.716  1.00 36.72           C
ATOM   2311  CE1 TYR A 297      30.346  17.907  22.039  1.00 37.15           C
ATOM   2312  CE2 TYR A 297      32.423  16.747  22.226  1.00 35.89           C
ATOM   2313  CZ  TYR A 297      31.088  16.764  21.893  1.00 36.57           C
ATOM   2314  OH  TYR A 297      30.467  15.641  21.405  1.00 36.99           O
ATOM   2315  N   LYS A 298      34.696  21.303  26.039  1.00 37.93           N
ATOM   2316  CA  LYS A 298      35.615  22.347  26.495  1.00 38.45           C
ATOM   2317  C   LYS A 298      36.090  22.994  25.236  1.00 38.43           C
ATOM   2318  O   LYS A 298      36.245  22.320  24.229  1.00 38.55           O
ATOM   2319  CB  LYS A 298      36.835  21.782  27.233  1.00 38.67           C
ATOM   2320  CG  LYS A 298      36.634  21.550  28.737  1.00 40.58           C
ATOM   2321  CD  LYS A 298      37.928  21.093  29.484  1.00 42.63           C
ATOM   2322  CE  LYS A 298      37.631  20.622  30.951  1.00 44.00           C
ATOM   2323  NZ  LYS A 298      38.841  20.251  31.812  1.00 43.61           N
ATOM   2324  N   GLY A 299      36.347  24.286  25.277  1.00 38.82           N
ATOM   2325  CA  GLY A 299      36.768  24.976  24.080  1.00 39.19           C
ATOM   2326  C   GLY A 299      38.174  24.582  23.719  1.00 39.60           C
ATOM   2327  O   GLY A 299      38.859  23.930  24.502  1.00 39.93           O
ATOM   2328  N   ALA A 300      38.594  24.963  22.520  1.00 40.20           N
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|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2329 | CA | ALA A 300 | 39.963 | 24.751 | 22.072 | 1.00 | 40.70 | C |
| ATOM | 2330 | C | ALA A 300 | 40.917 | 25.588 | 22.929 | 1.00 | 41.18 | C |
| ATOM | 2331 | O | ALA A 300 | 40.483 | 26.417 | 23.722 | 1.00 | 41.25 | O |
| ATOM | 2332 | CB | ALA A 300 | 40.085 | 25.143 | 20.616 | 1.00 | 40.64 | C |
| ATOM | 2333 | N | PRO A 301 | 42.215 | 25.408 | 22.733 | 1.00 | 41.91 | N |
| ATOM | 2334 | CA | PRO A 301 | 43.213 | 26.102 | 23.542 | 1.00 | 42.49 | C |
| ATOM | 2335 | C | PRO A 301 | 43.448 | 27.541 | 23.128 | 1.00 | 43.14 | C |
| ATOM | 2336 | O | PRO A 301 | 43.323 | 27.899 | 21.962 | 1.00 | 43.31 | O |
| ATOM | 2337 | CB | PRO A 301 | 44.483 | 25.326 | 23.230 | 1.00 | 42.38 | C |
| ATOM | 2338 | CG | PRO A 301 | 44.300 | 24.924 | 21.833 | 1.00 | 42.16 | C |
| ATOM | 2339 | CD | PRO A 301 | 42.851 | 24.571 | 21.701 | 1.00 | 41.99 | C |
| ATOM | 2340 | N | THR A 302 | 43.823 | 28.343 | 24.112 | 1.00 | 43.86 | N |
| ATOM | 2341 | CA | THR A 302 | 44.199 | 29.726 | 23.915 | 1.00 | 44.26 | C |
| ATOM | 2342 | C | THR A 302 | 45.588 | 29.732 | 23.318 | 1.00 | 44.56 | C |
| ATOM | 2343 | O | THR A 302 | 46.524 | 29.337 | 24.011 | 1.00 | 44.82 | O |
| ATOM | 2344 | CB | THR A 302 | 44.284 | 30.383 | 25.277 | 1.00 | 44.20 | C |
| ATOM | 2345 | OG1 | THR A 302 | 43.030 | 30.253 | 25.956 | 1.00 | 45.23 | O |
| ATOM | 2346 | CG2 | THR A 302 | 44.512 | 31.858 | 25.138 | 1.00 | 44.53 | C |
| ATOM | 2347 | N | PRO A 303 | 45.770 | 30.229 | 22.091 | 1.00 | 44.72 | N |
| ATOM | 2348 | CA | PRO A 303 | 47.083 | 30.128 | 21.438 | 1.00 | 44.51 | C |
| ATOM | 2349 | C | PRO A 303 | 48.177 | 30.759 | 22.306 | 1.00 | 44.48 | C |
| ATOM | 2350 | O | PRO A 303 | 47.835 | 31.522 | 23.221 | 1.00 | 44.02 | O |
| ATOM | 2351 | CB | PRO A 303 | 46.897 | 30.929 | 20.145 | 1.00 | 44.55 | C |
| ATOM | 2352 | CG | PRO A 303 | 45.426 | 30.929 | 19.904 | 1.00 | 44.28 | C |
| ATOM | 2353 | CD | PRO A 303 | 44.834 | 31.040 | 21.288 | 1.00 | 44.71 | C |
| ATOM | 2354 | N | GLU A 307 | 46.829 | 36.983 | 18.732 | 1.00 | 42.48 | N |
| ATOM | 2355 | CA | GLU A 307 | 46.845 | 37.952 | 17.646 | 1.00 | 42.70 | C |
| ATOM | 2356 | C | GLU A 307 | 45.812 | 39.039 | 17.801 | 1.00 | 42.57 | C |
| ATOM | 2357 | O | GLU A 307 | 44.654 | 38.807 | 18.138 | 1.00 | 42.62 | O |
| ATOM | 2358 | CB | GLU A 307 | 46.624 | 37.296 | 16.284 | 1.00 | 43.00 | C |
| ATOM | 2359 | CG | GLU A 307 | 46.980 | 38.235 | 15.127 | 1.00 | 43.85 | C |
| ATOM | 2360 | CD | GLU A 307 | 47.091 | 37.541 | 13.779 | 1.00 | 44.71 | C |
| ATOM | 2361 | OE1 | GLU A 307 | 46.618 | 36.385 | 13.643 | 1.00 | 45.10 | O |
| ATOM | 2362 | OE2 | GLU A 307 | 47.649 | 38.170 | 12.851 | 1.00 | 45.60 | O |
| ATOM | 2363 | N | TYR A 308 | 46.249 | 40.243 | 17.503 | 1.00 | 42.66 | N |
| ATOM | 2364 | CA | TYR A 308 | 45.384 | 41.379 | 17.577 | 1.00 | 42.64 | C |
| ATOM | 2365 | C | TYR A 308 | 44.814 | 41.530 | 16.189 | 1.00 | 42.85 | C |
| ATOM | 2366 | O | TYR A 308 | 45.413 | 41.066 | 15.203 | 1.00 | 43.43 | O |
| ATOM | 2367 | CB | TYR A 308 | 46.184 | 42.565 | 18.034 | 1.00 | 42.47 | C |
| ATOM | 2368 | CG | TYR A 308 | 46.744 | 42.281 | 19.399 | 1.00 | 43.35 | C |
| ATOM | 2369 | CD1 | TYR A 308 | 45.996 | 42.552 | 20.534 | 1.00 | 44.58 | C |
| ATOM | 2370 | CD2 | TYR A 308 | 47.986 | 41.681 | 19.559 | 1.00 | 43.97 | C |
| ATOM | 2371 | CE1 | TYR A 308 | 46.482 | 42.284 | 21.790 | 1.00 | 45.23 | C |
| ATOM | 2372 | CE2 | TYR A 308 | 48.483 | 41.401 | 20.818 | 1.00 | 44.79 | C |
| ATOM | 2373 | CZ | TYR A 308 | 47.726 | 41.708 | 21.935 | 1.00 | 45.46 | C |
| ATOM | 2374 | OH | TYR A 308 | 48.200 | 41.453 | 23.207 | 1.00 | 45.86 | O |
| ATOM | 2375 | N | PRO A 309 | 43.631 | 42.119 | 16.111 | 1.00 | 42.47 | N |
| ATOM | 2376 | CA | PRO A 309 | 42.930 | 42.648 | 17.285 | 1.00 | 42.08 | C |
| ATOM | 2377 | C | PRO A 309 | 42.209 | 41.528 | 18.051 | 1.00 | 41.24 | C |
| ATOM | 2378 | O | PRO A 309 | 41.774 | 40.578 | 17.408 | 1.00 | 40.92 | O |
| ATOM | 2379 | CB | PRO A 309 | 41.910 | 43.583 | 16.652 | 1.00 | 42.39 | C |
| ATOM | 2380 | CG | PRO A 309 | 41.574 | 42.895 | 15.337 | 1.00 | 42.16 | C |
| ATOM | 2381 | CD | PRO A 309 | 42.843 | 42.260 | 14.874 | 1.00 | 42.28 | C |
| ATOM | 2382 | N | LEU A 310 | 42.059 | 41.654 | 19.372 | 1.00 | 40.25 | N |
| ATOM | 2383 | CA | LEU A 310 | 41.436 | 40.596 | 20.180 | 1.00 | 39.46 | C |
| ATOM | 2384 | C | LEU A 310 | 39.971 | 40.434 | 19.884 | 1.00 | 38.93 | C |
| ATOM | 2385 | O | LEU A 310 | 39.288 | 41.412 | 19.624 | 1.00 | 39.65 | O |
| ATOM | 2386 | CB | LEU A 310 | 41.526 | 40.916 | 21.658 | 1.00 | 39.21 | C |
| ATOM | 2387 | CG | LEU A 310 | 42.486 | 40.099 | 22.508 | 1.00 | 38.87 | C |
| ATOM | 2388 | CD1 | LEU A 310 | 43.727 | 39.738 | 21.750 | 1.00 | 38.58 | C |
| ATOM | 2389 | CD2 | LEU A 310 | 42.817 | 40.926 | 23.735 | 1.00 | 39.01 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2390 | N | LYS | A | 311 | 39.462 | 39.217 | 19.957 | 1.00 | 37.90 | N |
| ATOM | 2391 | CA | LYS | A | 311 | 38.036 | 39.029 | 19.731 | 1.00 | 37.53 | C |
| ATOM | 2392 | C | LYS | A | 311 | 37.217 | 39.359 | 20.978 | 1.00 | 36.85 | C |
| ATOM | 2393 | O | LYS | A | 311 | 37.705 | 39.272 | 22.092 | 1.00 | 36.85 | O |
| ATOM | 2394 | CB | LYS | A | 311 | 37.746 | 37.609 | 19.274 | 1.00 | 37.54 | C |
| ATOM | 2395 | N | ALA | A | 312 | 35.965 | 39.736 | 20.793 | 1.00 | 36.18 | N |
| ATOM | 2396 | CA | ALA | A | 312 | 35.112 | 40.015 | 21.937 | 1.00 | 35.92 | C |
| ATOM | 2397 | C | ALA | A | 312 | 35.232 | 38.994 | 23.058 | 1.00 | 35.88 | C |
| ATOM | 2398 | O | ALA | A | 312 | 35.347 | 39.384 | 24.213 | 1.00 | 35.99 | O |
| ATOM | 2399 | CB | ALA | A | 312 | 33.665 | 40.115 | 21.526 | 1.00 | 35.50 | C |
| ATOM | 2400 | N | HIS | A | 313 | 35.221 | 37.700 | 22.739 | 1.00 | 35.71 | N |
| ATOM | 2401 | CA | HIS | A | 313 | 35.136 | 36.709 | 23.797 | 1.00 | 35.52 | C |
| ATOM | 2402 | C | HIS | A | 313 | 36.429 | 36.694 | 24.517 | 1.00 | 35.31 | C |
| ATOM | 2403 | O | HIS | A | 313 | 36.489 | 36.278 | 25.667 | 1.00 | 35.53 | O |
| ATOM | 2404 | CB | HIS | A | 313 | 34.768 | 35.291 | 23.313 | 1.00 | 35.89 | C |
| ATOM | 2405 | CG | HIS | A | 313 | 35.844 | 34.613 | 22.535 | 1.00 | 36.41 | C |
| ATOM | 2406 | ND1 | HIS | A | 313 | 36.097 | 34.905 | 21.214 | 1.00 | 38.71 | N |
| ATOM | 2407 | CD2 | HIS | A | 313 | 36.741 | 33.665 | 22.889 | 1.00 | 37.90 | C |
| ATOM | 2408 | CE1 | HIS | A | 313 | 37.111 | 34.175 | 20.789 | 1.00 | 38.65 | C |
| ATOM | 2409 | NE2 | HIS | A | 313 | 37.524 | 33.416 | 21.788 | 1.00 | 38.60 | N |
| ATOM | 2410 | N | GLN | A | 314 | 37.478 | 37.162 | 23.861 | 1.00 | 35.08 | N |
| ATOM | 2411 | CA | GLN | A | 314 | 38.760 | 37.203 | 24.535 | 1.00 | 35.00 | C |
| ATOM | 2412 | C | GLN | A | 314 | 38.706 | 38.301 | 25.576 | 1.00 | 34.62 | C |
| ATOM | 2413 | O | GLN | A | 314 | 39.145 | 38.109 | 26.703 | 1.00 | 34.28 | O |
| ATOM | 2414 | CB | GLN | A | 314 | 39.924 | 37.399 | 23.558 | 1.00 | 35.10 | C |
| ATOM | 2415 | CG | GLN | A | 314 | 40.091 | 36.229 | 22.597 | 1.00 | 35.42 | C |
| ATOM | 2416 | CD | GLN | A | 314 | 41.107 | 36.478 | 21.500 | 1.00 | 35.10 | C |
| ATOM | 2417 | OE1 | GLN | A | 314 | 40.938 | 37.377 | 20.671 | 1.00 | 35.86 | O |
| ATOM | 2418 | NE2 | GLN | A | 314 | 42.150 | 35.666 | 21.476 | 1.00 | 34.32 | N |
| ATOM | 2419 | N | LYS | A | 315 | 38.173 | 39.454 | 25.197 | 1.00 | 34.70 | N |
| ATOM | 2420 | CA | LYS | A | 315 | 38.009 | 40.539 | 26.152 | 1.00 | 35.01 | C |
| ATOM | 2421 | C | LYS | A | 315 | 37.164 | 40.063 | 27.320 | 1.00 | 34.67 | C |
| ATOM | 2422 | O | LYS | A | 315 | 37.485 | 40.325 | 28.467 | 1.00 | 34.81 | O |
| ATOM | 2423 | CB | LYS | A | 315 | 37.395 | 41.766 | 25.501 | 1.00 | 35.19 | C |
| ATOM | 2424 | CG | LYS | A | 315 | 38.344 | 42.447 | 24.563 | 1.00 | 35.85 | C |
| ATOM | 2425 | CD | LYS | A | 315 | 37.703 | 43.636 | 23.931 | 1.00 | 37.25 | C |
| ATOM | 2426 | CE | LYS | A | 315 | 38.657 | 44.348 | 23.001 | 1.00 | 39.28 | C |
| ATOM | 2427 | NZ | LYS | A | 315 | 37.969 | 45.430 | 22.222 | 1.00 | 40.34 | N |
| ATOM | 2428 | N | VAL | A | 316 | 36.117 | 39.314 | 27.040 | 1.00 | 34.30 | N |
| ATOM | 2429 | CA | VAL | A | 316 | 35.321 | 38.787 | 28.118 | 1.00 | 34.31 | C |
| ATOM | 2430 | C | VAL | A | 316 | 36.175 | 37.925 | 29.047 | 1.00 | 34.37 | C |
| ATOM | 2431 | O | VAL | A | 316 | 36.071 | 38.023 | 30.273 | 1.00 | 34.57 | O |
| ATOM | 2432 | CB | VAL | A | 316 | 34.138 | 37.992 | 27.606 | 1.00 | 34.39 | C |
| ATOM | 2433 | CG1 | VAL | A | 316 | 33.334 | 37.434 | 28.794 | 1.00 | 34.91 | C |
| ATOM | 2434 | CG2 | VAL | A | 316 | 33.258 | 38.873 | 26.719 | 1.00 | 33.60 | C |
| ATOM | 2435 | N | ALA | A | 317 | 37.011 | 37.072 | 28.475 | 1.00 | 34.24 | N |
| ATOM | 2436 | CA | ALA | A | 317 | 37.907 | 36.267 | 29.288 | 1.00 | 34.17 | C |
| ATOM | 2437 | C | ALA | A | 317 | 38.744 | 37.160 | 30.166 | 1.00 | 34.10 | C |
| ATOM | 2438 | O | ALA | A | 317 | 38.919 | 36.906 | 31.352 | 1.00 | 33.87 | O |
| ATOM | 2439 | CB | ALA | A | 317 | 38.813 | 35.459 | 28.431 | 1.00 | 34.02 | C |
| ATOM | 2440 | N | ILE | A | 318 | 39.274 | 38.216 | 29.574 | 1.00 | 34.29 | N |
| ATOM | 2441 | CA | ILE | A | 318 | 40.178 | 39.062 | 30.322 | 1.00 | 34.26 | C |
| ATOM | 2442 | C | ILE | A | 318 | 39.467 | 39.611 | 31.546 | 1.00 | 33.99 | C |
| ATOM | 2443 | O | ILE | A | 318 | 39.993 | 39.556 | 32.661 | 1.00 | 33.96 | O |
| ATOM | 2444 | CB | ILE | A | 318 | 40.755 | 40.171 | 29.447 | 1.00 | 33.98 | C |
| ATOM | 2445 | CG1 | ILE | A | 318 | 41.775 | 39.558 | 28.489 | 1.00 | 34.02 | C |
| ATOM | 2446 | CG2 | ILE | A | 318 | 41.429 | 41.188 | 30.323 | 1.00 | 33.92 | C |
| ATOM | 2447 | CD1 | ILE | A | 318 | 42.356 | 40.498 | 27.428 | 1.00 | 33.97 | C |
| ATOM | 2448 | N | MET | A | 319 | 38.241 | 40.068 | 31.337 | 1.00 | 33.55 | N |
| ATOM | 2449 | CA | MET | A | 319 | 37.499 | 40.741 | 32.383 | 1.00 | 33.41 | C |
| ATOM | 2450 | C | MET | A | 319 | 37.196 | 39.772 | 33.496 | 1.00 | 33.38 | C |

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|---|---|---|---|---|---|---|---|---|---|---|
| ATOM | 2451 | O | MET | A | 319 | 37.238 | 40.101 | 34.669 | 1.00 | 33.32 | O |
| ATOM | 2452 | CB | MET | A | 319 | 36.193 | 41.308 | 31.827 | 1.00 | 33.31 | C |
| ATOM | 2453 | CG | MET | A | 319 | 36.361 | 42.521 | 30.951 | 1.00 | 32.96 | C |
| ATOM | 2454 | SD | MET | A | 319 | 34.812 | 43.355 | 30.617 | 1.00 | 33.05 | S |
| ATOM | 2455 | CE | MET | A | 319 | 34.119 | 42.299 | 29.410 | 1.00 | 33.43 | C |
| ATOM | 2456 | N | ARG | A | 320 | 36.873 | 38.558 | 33.121 | 1.00 | 33.68 | N |
| ATOM | 2457 | CA | ARG | A | 320 | 36.575 | 37.568 | 34.112 | 1.00 | 33.61 | C |
| ATOM | 2458 | C | ARG | A | 320 | 37.796 | 37.392 | 34.996 | 1.00 | 33.82 | C |
| ATOM | 2459 | O | ARG | A | 320 | 37.719 | 37.448 | 36.225 | 1.00 | 33.48 | O |
| ATOM | 2460 | CB | ARG | A | 320 | 36.211 | 36.292 | 33.402 | 1.00 | 33.39 | C |
| ATOM | 2461 | CG | ARG | A | 320 | 34.875 | 36.406 | 32.725 | 1.00 | 33.88 | C |
| ATOM | 2462 | CD | ARG | A | 320 | 34.268 | 35.080 | 32.340 | 1.00 | 34.20 | C |
| ATOM | 2463 | NE | ARG | A | 320 | 34.217 | 34.215 | 33.507 | 1.00 | 33.14 | N |
| ATOM | 2464 | CZ | ARG | A | 320 | 33.159 | 34.103 | 34.260 | 1.00 | 33.15 | C |
| ATOM | 2465 | NH1 | ARG | A | 320 | 32.077 | 34.762 | 33.933 | 1.00 | 33.83 | N |
| ATOM | 2466 | NH2 | ARG | A | 320 | 33.170 | 33.338 | 35.331 | 1.00 | 34.46 | N |
| ATOM | 2467 | N | ASN | A | 321 | 38.941 | 37.232 | 34.355 | 1.00 | 33.92 | N |
| ATOM | 2468 | CA | ASN | A | 321 | 40.143 | 36.978 | 35.085 | 1.00 | 34.08 | C |
| ATOM | 2469 | C | ASN | A | 321 | 40.486 | 38.141 | 36.018 | 1.00 | 34.26 | C |
| ATOM | 2470 | O | ASN | A | 321 | 40.874 | 37.919 | 37.164 | 1.00 | 34.14 | O |
| ATOM | 2471 | CB | ASN | A | 321 | 41.271 | 36.616 | 34.119 | 1.00 | 34.30 | C |
| ATOM | 2472 | CG | ASN | A | 321 | 41.195 | 35.161 | 33.663 | 1.00 | 34.44 | C |
| ATOM | 2473 | OD1 | ASN | A | 321 | 40.829 | 34.273 | 34.434 | 1.00 | 34.16 | O |
| ATOM | 2474 | ND2 | ASN | A | 321 | 41.522 | 34.918 | 32.402 | 1.00 | 35.05 | N |
| ATOM | 2475 | N | ILE | A | 322 | 40.318 | 39.379 | 35.569 | 1.00 | 34.24 | N |
| ATOM | 2476 | CA | ILE | A | 322 | 40.634 | 40.488 | 36.448 | 1.00 | 34.25 | C |
| ATOM | 2477 | C | ILE | A | 322 | 39.781 | 40.408 | 37.701 | 1.00 | 33.85 | C |
| ATOM | 2478 | O | ILE | A | 322 | 40.250 | 40.711 | 38.789 | 1.00 | 34.16 | O |
| ATOM | 2479 | CB | ILE | A | 322 | 40.412 | 41.837 | 35.760 | 1.00 | 34.70 | C |
| ATOM | 2480 | CG1 | ILE | A | 322 | 41.338 | 41.993 | 34.558 | 1.00 | 35.34 | C |
| ATOM | 2481 | CG2 | ILE | A | 322 | 40.651 | 43.007 | 36.748 | 1.00 | 35.37 | C |
| ATOM | 2482 | CD1 | ILE | A | 322 | 42.778 | 41.928 | 34.895 | 1.00 | 36.17 | C |
| ATOM | 2483 | N | GLU | A | 323 | 38.525 | 40.013 | 37.558 | 1.00 | 33.42 | N |
| ATOM | 2484 | CA | GLU | A | 323 | 37.636 | 39.935 | 38.704 | 1.00 | 32.97 | C |
| ATOM | 2485 | C | GLU | A | 323 | 38.085 | 38.842 | 39.652 | 1.00 | 33.11 | C |
| ATOM | 2486 | O | GLU | A | 323 | 38.067 | 39.001 | 40.864 | 1.00 | 32.66 | O |
| ATOM | 2487 | CB | GLU | A | 323 | 36.199 | 39.673 | 38.256 | 1.00 | 32.73 | C |
| ATOM | 2488 | CG | GLU | A | 323 | 35.543 | 40.907 | 37.672 | 1.00 | 33.02 | C |
| ATOM | 2489 | CD | GLU | A | 323 | 34.166 | 40.693 | 37.057 | 1.00 | 32.91 | C |
| ATOM | 2490 | OE1 | GLU | A | 323 | 33.193 | 40.309 | 37.740 | 1.00 | 31.94 | O |
| ATOM | 2491 | OE2 | GLU | A | 323 | 34.048 | 40.961 | 35.856 | 1.00 | 33.81 | O |
| ATOM | 2492 | N | LYS | A | 324 | 38.497 | 37.720 | 39.088 | 1.00 | 33.56 | N |
| ATOM | 2493 | CA | LYS | A | 324 | 38.882 | 36.588 | 39.895 | 1.00 | 33.72 | C |
| ATOM | 2494 | C | LYS | A | 324 | 40.138 | 36.937 | 40.670 | 1.00 | 34.09 | C |
| ATOM | 2495 | O | LYS | A | 324 | 40.228 | 36.664 | 41.859 | 1.00 | 34.15 | O |
| ATOM | 2496 | CB | LYS | A | 324 | 39.119 | 35.368 | 39.012 | 1.00 | 33.73 | C |
| ATOM | 2497 | CG | LYS | A | 324 | 37.877 | 34.766 | 38.353 | 1.00 | 33.83 | C |
| ATOM | 2498 | CD | LYS | A | 324 | 38.355 | 33.673 | 37.440 | 1.00 | 33.70 | C |
| ATOM | 2499 | CE | LYS | A | 324 | 37.294 | 32.883 | 36.723 | 1.00 | 33.57 | C |
| ATOM | 2500 | NZ | LYS | A | 324 | 37.993 | 31.761 | 35.984 | 1.00 | 32.76 | N |
| ATOM | 2501 | N | MET | A | 325 | 41.098 | 37.558 | 39.995 | 1.00 | 34.73 | N |
| ATOM | 2502 | CA | MET | A | 325 | 42.380 | 37.915 | 40.609 | 1.00 | 35.32 | C |
| ATOM | 2503 | C | MET | A | 325 | 42.248 | 38.883 | 41.766 | 1.00 | 35.06 | C |
| ATOM | 2504 | O | MET | A | 325 | 42.888 | 38.729 | 42.808 | 1.00 | 34.50 | O |
| ATOM | 2505 | CB | MET | A | 325 | 43.328 | 38.501 | 39.563 | 1.00 | 35.57 | C |
| ATOM | 2506 | CG | MET | A | 325 | 43.962 | 37.419 | 38.724 | 1.00 | 36.96 | C |
| ATOM | 2507 | SD | MET | A | 325 | 44.984 | 37.973 | 37.360 | 1.00 | 40.43 | S |
| ATOM | 2508 | CE | MET | A | 325 | 45.710 | 39.363 | 38.037 | 1.00 | 41.05 | C |
| ATOM | 2509 | N | LEU | A | 326 | 41.427 | 39.891 | 41.555 | 1.00 | 35.32 | N |
| ATOM | 2510 | CA | LEU | A | 326 | 41.178 | 40.895 | 42.570 | 1.00 | 35.83 | C |
| ATOM | 2511 | C | LEU | A | 326 | 40.556 | 40.230 | 43.770 | 1.00 | 35.60 | C |

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ATOM   2512  O   LEU A 326      40.914  40.507  44.910  1.00 35.34           O
ATOM   2513  CB  LEU A 326      40.216  41.929  42.026  1.00 36.07           C
ATOM   2514  CG  LEU A 326      40.721  43.321  41.689  1.00 37.48           C
ATOM   2515  CD1 LEU A 326      42.221  43.442  41.537  1.00 38.59           C
ATOM   2516  CD2 LEU A 326      40.049  43.692  40.413  1.00 38.65           C
ATOM   2517  N   GLY A 327      39.613  39.341  43.493  1.00 35.59           N
ATOM   2518  CA  GLY A 327      38.947  38.604  44.538  1.00 35.54           C
ATOM   2519  C   GLY A 327      39.983  37.998  45.443  1.00 35.62           C
ATOM   2520  O   GLY A 327      40.023  38.258  46.641  1.00 35.52           O
ATOM   2521  N   GLU A 328      40.863  37.209  44.851  1.00 35.84           N
ATOM   2522  CA  GLU A 328      41.831  36.486  45.632  1.00 35.91           C
ATOM   2523  C   GLU A 328      42.783  37.424  46.298  1.00 35.44           C
ATOM   2524  O   GLU A 328      43.086  37.272  47.465  1.00 35.60           O
ATOM   2525  CB  GLU A 328      42.584  35.513  44.750  1.00 36.21           C
ATOM   2526  CG  GLU A 328      41.675  34.419  44.226  1.00 38.20           C
ATOM   2527  CD  GLU A 328      41.854  33.088  44.941  1.00 41.33           C
ATOM   2528  OE1 GLU A 328      42.244  33.084  46.138  1.00 42.40           O
ATOM   2529  OE2 GLU A 328      41.608  32.034  44.292  1.00 43.59           O
ATOM   2530  N   ALA A 329      43.220  38.435  45.577  1.00 35.11           N
ATOM   2531  CA  ALA A 329      44.259  39.282  46.110  1.00 34.85           C
ATOM   2532  C   ALA A 329      43.790  40.103  47.296  1.00 34.75           C
ATOM   2533  O   ALA A 329      44.533  40.282  48.258  1.00 34.53           O
ATOM   2534  CB  ALA A 329      44.778  40.163  45.046  1.00 34.85           C
ATOM   2535  N   LEU A 330      42.567  40.613  47.214  1.00 34.62           N
ATOM   2536  CA  LEU A 330      41.996  41.399  48.291  1.00 34.55           C
ATOM   2537  C   LEU A 330      41.478  40.555  49.448  1.00 34.90           C
ATOM   2538  O   LEU A 330      41.234  41.072  50.532  1.00 35.33           O
ATOM   2539  CB  LEU A 330      40.851  42.245  47.766  1.00 34.31           C
ATOM   2540  CG  LEU A 330      41.202  43.322  46.743  1.00 34.06           C
ATOM   2541  CD1 LEU A 330      39.942  43.965  46.258  1.00 34.23           C
ATOM   2542  CD2 LEU A 330      42.078  44.382  47.285  1.00 34.05           C
ATOM   2543  N   GLY A 331      41.295  39.262  49.232  1.00 35.23           N
ATOM   2544  CA  GLY A 331      40.794  38.401  50.285  1.00 35.49           C
ATOM   2545  C   GLY A 331      39.306  38.471  50.584  1.00 35.66           C
ATOM   2546  O   GLY A 331      38.849  37.859  51.544  1.00 35.61           O
ATOM   2547  N   ASN A 332      38.547  39.213  49.790  1.00 36.04           N
ATOM   2548  CA  ASN A 332      37.113  39.295  49.992  1.00 36.44           C
ATOM   2549  C   ASN A 332      36.483  39.791  48.732  1.00 36.55           C
ATOM   2550  O   ASN A 332      36.647  40.951  48.381  1.00 37.01           O
ATOM   2551  CB  ASN A 332      36.775  40.275  51.094  1.00 36.54           C
ATOM   2552  CG  ASN A 332      35.311  40.260  51.440  1.00 37.47           C
ATOM   2553  OD1 ASN A 332      34.519  39.541  50.828  1.00 37.83           O
ATOM   2554  ND2 ASN A 332      34.938  41.043  52.444  1.00 39.90           N
ATOM   2555  N   PRO A 333      35.699  38.957  48.078  1.00 36.46           N
ATOM   2556  CA  PRO A 333      35.178  39.338  46.775  1.00 36.43           C
ATOM   2557  C   PRO A 333      34.368  40.590  46.908  1.00 36.32           C
ATOM   2558  O   PRO A 333      34.318  41.384  45.988  1.00 36.36           O
ATOM   2559  CB  PRO A 333      34.278  38.170  46.366  1.00 36.50           C
ATOM   2560  CG  PRO A 333      34.247  37.229  47.489  1.00 36.58           C
ATOM   2561  CD  PRO A 333      35.180  37.668  48.548  1.00 36.54           C
ATOM   2562  N   GLN A 334      33.743  40.800  48.047  1.00 36.44           N
ATOM   2563  CA  GLN A 334      32.906  41.969  48.130  1.00 36.85           C
ATOM   2564  C   GLN A 334      33.748  43.222  48.057  1.00 36.57           C
ATOM   2565  O   GLN A 334      33.218  44.304  47.868  1.00 36.98           O
ATOM   2566  CB  GLN A 334      31.987  41.940  49.348  1.00 37.31           C
ATOM   2567  CG  GLN A 334      30.685  41.151  49.026  1.00 38.95           C
ATOM   2568  CD  GLN A 334      29.669  41.097  50.171  1.00 40.33           C
ATOM   2569  OE1 GLN A 334      29.751  41.872  51.137  1.00 41.70           O
ATOM   2570  NE2 GLN A 334      28.712  40.178  50.061  1.00 39.80           N
ATOM   2571  N   GLU A 335      35.064  43.088  48.159  1.00 35.99           N
ATOM   2572  CA  GLU A 335      35.914  44.261  48.067  1.00 35.53           C
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ATOM   2573  C   GLU A 335      36.229  44.610  46.621  1.00 34.53           C
ATOM   2574  O   GLU A 335      36.715  45.689  46.338  1.00 34.20           O
ATOM   2575  CB  GLU A 335      37.201  44.083  48.894  1.00 35.99           C
ATOM   2576  CG  GLU A 335      37.054  44.507  50.354  1.00 37.38           C
ATOM   2577  CD  GLU A 335      38.382  44.592  51.076  1.00 40.16           C
ATOM   2578  OE1 GLU A 335      39.271  45.318  50.570  1.00 42.04           O
ATOM   2579  OE2 GLU A 335      38.535  43.952  52.153  1.00 41.52           O
ATOM   2580  N   VAL A 336      35.922  43.701  45.706  1.00 33.97           N
ATOM   2581  CA  VAL A 336      36.165  43.901  44.276  1.00 33.49           C
ATOM   2582  C   VAL A 336      35.537  45.159  43.670  1.00 33.00           C
ATOM   2583  O   VAL A 336      36.194  45.904  42.946  1.00 33.01           O
ATOM   2584  CB  VAL A 336      35.696  42.678  43.473  1.00 33.36           C
ATOM   2585  CG1 VAL A 336      35.726  42.951  41.992  1.00 34.05           C
ATOM   2586  CG2 VAL A 336      36.582  41.509  43.755  1.00 33.01           C
ATOM   2587  N   GLY A 337      34.270  45.406  43.926  1.00 32.41           N
ATOM   2588  CA  GLY A 337      33.675  46.592  43.351  1.00 32.21           C
ATOM   2589  C   GLY A 337      34.332  47.903  43.724  1.00 31.72           C
ATOM   2590  O   GLY A 337      34.682  48.711  42.859  1.00 31.40           O
ATOM   2591  N   PRO A 338      34.433  48.163  45.013  1.00 31.50           N
ATOM   2592  CA  PRO A 338      35.025  49.415  45.470  1.00 31.47           C
ATOM   2593  C   PRO A 338      36.387  49.648  44.846  1.00 31.60           C
ATOM   2594  O   PRO A 338      36.655  50.756  44.386  1.00 31.51           O
ATOM   2595  CB  PRO A 338      35.065  49.230  46.977  1.00 31.27           C
ATOM   2596  CG  PRO A 338      33.883  48.376  47.218  1.00 31.08           C
ATOM   2597  CD  PRO A 338      33.933  47.359  46.137  1.00 31.28           C
ATOM   2598  N   LEU A 339      37.219  48.620  44.765  1.00 31.80           N
ATOM   2599  CA  LEU A 339      38.531  48.825  44.182  1.00 32.25           C
ATOM   2600  C   LEU A 339      38.431  49.269  42.740  1.00 32.12           C
ATOM   2601  O   LEU A 339      39.130  50.188  42.320  1.00 32.25           O
ATOM   2602  CB  LEU A 339      39.395  47.581  44.278  1.00 32.49           C
ATOM   2603  CG  LEU A 339      40.853  47.920  43.962  1.00 33.78           C
ATOM   2604  CD1 LEU A 339      41.793  47.121  44.797  1.00 34.64           C
ATOM   2605  CD2 LEU A 339      41.146  47.681  42.516  1.00 34.50           C
ATOM   2606  N   LEU A 340      37.567  48.607  41.978  1.00 32.12           N
ATOM   2607  CA  LEU A 340      37.385  48.963  40.584  1.00 31.85           C
ATOM   2608  C   LEU A 340      36.854  50.376  40.483  1.00 31.56           C
ATOM   2609  O   LEU A 340      37.342  51.169  39.701  1.00 31.42           O
ATOM   2610  CB  LEU A 340      36.468  47.975  39.888  1.00 31.90           C
ATOM   2611  CG  LEU A 340      37.089  46.598  39.669  1.00 32.44           C
ATOM   2612  CD1 LEU A 340      36.028  45.636  39.132  1.00 33.11           C
ATOM   2613  CD2 LEU A 340      38.281  46.660  38.728  1.00 31.95           C
ATOM   2614  N   ASN A 341      35.865  50.717  41.282  1.00 31.61           N
ATOM   2615  CA  ASN A 341      35.384  52.083  41.231  1.00 31.82           C
ATOM   2616  C   ASN A 341      36.484  53.109  41.525  1.00 31.45           C
ATOM   2617  O   ASN A 341      36.600  54.119  40.845  1.00 30.80           O
ATOM   2618  CB  ASN A 341      34.212  52.260  42.177  1.00 31.97           C
ATOM   2619  CG  ASN A 341      32.901  51.883  41.532  1.00 32.77           C
ATOM   2620  OD1 ASN A 341      32.426  52.568  40.614  1.00 34.75           O
ATOM   2621  ND2 ASN A 341      32.310  50.789  41.992  1.00 31.86           N
ATOM   2622  N   THR A 342      37.301  52.835  42.530  1.00 31.40           N
ATOM   2623  CA  THR A 342      38.380  53.739  42.880  1.00 31.27           C
ATOM   2624  C   THR A 342      39.317  53.842  41.707  1.00 31.14           C
ATOM   2625  O   THR A 342      39.837  54.908  41.402  1.00 30.66           O
ATOM   2626  CB  THR A 342      39.146  53.217  44.097  1.00 31.43           C
ATOM   2627  OG1 THR A 342      38.448  53.565  45.299  1.00 30.95           O
ATOM   2628  CG2 THR A 342      40.500  53.913  44.228  1.00 31.17           C
ATOM   2629  N   MET A 343      39.549  52.714  41.059  1.00 31.29           N
ATOM   2630  CA  MET A 343      40.406  52.703  39.898  1.00 31.59           C
ATOM   2631  C   MET A 343      39.970  53.639  38.785  1.00 31.49           C
ATOM   2632  O   MET A 343      40.804  54.361  38.255  1.00 31.46           O
ATOM   2633  CB  MET A 343      40.516  51.310  39.314  1.00 31.79           C
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ATOM   2634  CG  MET A 343      41.831  50.662  39.629  1.00 32.65           C
ATOM   2635  SD  MET A 343      42.271  49.379  38.468  1.00 33.09           S
ATOM   2636  CE  MET A 343      41.116  48.304  38.916  1.00 34.22           C
ATOM   2637  N   ILE A 344      38.690  53.641  38.418  1.00 31.31           N
ATOM   2638  CA  ILE A 344      38.293  54.432  37.265  1.00 31.42           C
ATOM   2639  C   ILE A 344      37.708  55.787  37.533  1.00 31.14           C
ATOM   2640  O   ILE A 344      37.752  56.630  36.640  1.00 31.01           O
ATOM   2641  CB  ILE A 344      37.272  53.708  36.362  1.00 31.86           C
ATOM   2642  CG1 ILE A 344      35.870  53.866  36.928  1.00 33.16           C
ATOM   2643  CG2 ILE A 344      37.633  52.229  36.118  1.00 32.09           C
ATOM   2644  CD1 ILE A 344      34.876  53.232  36.072  1.00 35.18           C
ATOM   2645  N   LYS A 345      37.131  56.050  38.698  1.00 30.88           N
ATOM   2646  CA  LYS A 345      36.455  57.334  38.758  1.00 30.94           C
ATOM   2647  C   LYS A 345      37.412  58.468  38.853  1.00 30.72           C
ATOM   2648  O   LYS A 345      38.250  58.558  39.743  1.00 30.61           O
ATOM   2649  CB  LYS A 345      35.315  57.475  39.765  1.00 31.14           C
ATOM   2650  CG  LYS A 345      35.361  56.680  40.977  1.00 32.16           C
ATOM   2651  CD  LYS A 345      33.970  56.273  41.340  1.00 33.62           C
ATOM   2652  CE  LYS A 345      33.514  56.873  42.665  1.00 34.71           C
ATOM   2653  NZ  LYS A 345      34.302  56.317  43.840  1.00 36.28           N
ATOM   2654  N   GLY A 346      37.280  59.332  37.870  1.00 30.83           N
ATOM   2655  CA  GLY A 346      38.114  60.504  37.789  1.00 30.66           C
ATOM   2656  C   GLY A 346      39.345  60.195  37.001  1.00 30.25           C
ATOM   2657  O   GLY A 346      40.147  61.066  36.745  1.00 30.00           O
ATOM   2658  N   ARG A 347      39.454  58.953  36.564  1.00 30.42           N
ATOM   2659  CA  ARG A 347      40.652  58.496  35.923  1.00 30.66           C
ATOM   2660  C   ARG A 347      40.389  57.879  34.566  1.00 30.89           C
ATOM   2661  O   ARG A 347      41.033  58.241  33.588  1.00 30.30           O
ATOM   2662  CB  ARG A 347      41.350  57.526  36.860  1.00 30.88           C
ATOM   2663  CG  ARG A 347      41.786  58.177  38.171  1.00 30.97           C
ATOM   2664  CD  ARG A 347      43.129  57.701  38.636  1.00 31.35           C
ATOM   2665  NE  ARG A 347      43.128  56.255  38.597  1.00 30.88           N
ATOM   2666  CZ  ARG A 347      44.088  55.482  38.128  1.00 29.55           C
ATOM   2667  NH1 ARG A 347      45.237  55.962  37.667  1.00 28.44           N
ATOM   2668  NH2 ARG A 347      43.876  54.181  38.147  1.00 29.95           N
ATOM   2669  N   TYR A 348      39.446  56.953  34.480  1.00 31.67           N
ATOM   2670  CA  TYR A 348      39.143  56.377  33.176  1.00 32.27           C
ATOM   2671  C   TYR A 348      37.726  56.574  32.689  1.00 33.10           C
ATOM   2672  O   TYR A 348      37.425  56.212  31.557  1.00 33.12           O
ATOM   2673  CB  TYR A 348      39.422  54.896  33.154  1.00 31.96           C
ATOM   2674  CG  TYR A 348      40.860  54.527  33.253  1.00 32.06           C
ATOM   2675  CD1 TYR A 348      41.652  54.424  32.114  1.00 31.60           C
ATOM   2676  CD2 TYR A 348      41.435  54.256  34.483  1.00 31.75           C
ATOM   2677  CE1 TYR A 348      42.980  54.061  32.203  1.00 31.08           C
ATOM   2678  CE2 TYR A 348      42.761  53.897  34.580  1.00 32.11           C
ATOM   2679  CZ  TYR A 348      43.530  53.800  33.438  1.00 31.05           C
ATOM   2680  OH  TYR A 348      44.845  53.427  33.544  1.00 29.83           O
ATOM   2681  N   ASN A 349      36.850  57.137  33.507  1.00 34.48           N
ATOM   2682  CA  ASN A 349      35.465  57.275  33.083  1.00 35.73           C
ATOM   2683  C   ASN A 349      35.037  58.643  32.595  1.00 36.60           C
ATOM   2684  O   ASN A 349      35.757  59.640  32.508  1.00 37.31           O
ATOM   2685  CB  ASN A 349      34.542  56.900  34.212  1.00 35.62           C
ATOM   2686  CG  ASN A 349      34.635  57.864  35.353  1.00 37.08           C
ATOM   2687  OD1 ASN A 349      35.398  58.840  35.308  1.00 36.55           O
ATOM   2688  ND2 ASN A 349      33.861  57.604  36.403  1.00 39.78           N
ATOM   2689  OXT ASN A 349      33.861  58.757  32.276  1.00 38.11           O
TER    2690       ASN A 349
HETATM 2691  FE  FE2 A1350      23.364  27.586  28.889  1.00 32.45          FE
HETATM 2692  C1  AKG A1351      22.523  25.412  27.792  1.00 37.04           C
HETATM 2693  O1  AKG A1351      23.535  26.092  27.914  1.00 39.03           O
HETATM 2694  O2  AKG A1351      22.557  24.216  27.226  1.00 37.33           O
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HETATM 2695  C2  AKG A1351      21.186  25.964  28.297  1.00 35.25           C
HETATM 2696  O5  AKG A1351      21.175  27.063  28.807  1.00 33.44           O
HETATM 2697  C3  AKG A1351      19.937  25.139  28.167  1.00 36.11           C
HETATM 2698  C4  AKG A1351      18.848  25.738  29.055  1.00 36.50           C
HETATM 2699  C5  AKG A1351      17.464  25.331  28.632  1.00 35.97           C
HETATM 2700  O3  AKG A1351      17.276  24.627  27.656  1.00 36.64           O
HETATM 2701  O4  AKG A1351      16.432  25.771  29.338  1.00 36.31           O
HETATM 2702  S   SO4 A1352       0.300  25.196  43.477  1.00 80.75           S
HETATM 2703  O1  SO4 A1352       1.094  26.117  44.306  1.00 78.50           O
HETATM 2704  O2  SO4 A1352       1.221  24.413  42.644  1.00 78.51           O
HETATM 2705  O3  SO4 A1352      -0.470  24.282  44.334  1.00 79.54           O
HETATM 2706  O4  SO4 A1352      -0.640  25.951  42.633  1.00 78.07           O
HETATM 2707  S   SO4 A1353       1.825  28.603  29.515  1.00 77.38           S
HETATM 2708  O1  SO4 A1353       3.041  29.212  30.061  1.00 76.05           O
HETATM 2709  O2  SO4 A1353       2.144  27.528  28.574  1.00 75.24           O
HETATM 2710  O3  SO4 A1353       1.090  28.086  30.675  1.00 76.52           O
HETATM 2711  O4  SO4 A1353       1.011  29.586  28.783  1.00 76.04           O
HETATM 2712  S   SO4 A1354      34.403  30.284  38.043  1.00 78.17           S
HETATM 2713  O1  SO4 A1354      34.921  31.567  38.516  1.00 75.93           O
HETATM 2714  O2  SO4 A1354      35.240  29.158  38.450  1.00 77.42           O
HETATM 2715  O3  SO4 A1354      33.112  30.084  38.686  1.00 75.59           O
HETATM 2716  O4  SO4 A1354      34.303  30.307  36.581  1.00 74.60           O
HETATM 2717  O   HOH Z   1      25.824  26.442  26.175  1.00 46.43           O
HETATM 2718  O   HOH Z   2      27.811  27.709  24.637  1.00 41.32           O
HETATM 2719  O   HOH Z   3      27.367  30.233  25.742  1.00 38.18           O
CONECT 1478 2691
CONECT 1498 2691
CONECT 2167 2691
CONECT 2691 2696 2693 1478 2167 1498
CONECT 2692 2693 2694 2695
CONECT 2693 2692 2691
CONECT 2694 2692
CONECT 2695 2692 2696 2697
CONECT 2696 2691 2695
CONECT 2697 2695 2698
CONECT 2698 2697 2699
CONECT 2699 2698 2700 2701
CONECT 2700 2699
CONECT 2701 2699
CONECT 2702 2703 2704 2705 2706
CONECT 2703 2702
CONECT 2704 2702
CONECT 2705 2702
CONECT 2706 2702
CONECT 2707 2708 2709 2710 2711
CONECT 2708 2707
CONECT 2709 2707
CONECT 2710 2707
CONECT 2711 2707
CONECT 2712 2713 2714 2715 2716
CONECT 2713 2712
CONECT 2714 2712
CONECT 2715 2712
CONECT 2716 2712
MASTER      433    0    5   14   20    0    9    6 2718    1   29   27
END
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